

10/ 821,906

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:sssptal202txn

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * Welcome to STN International * * * * *

NEWS	1	Web Page URLs for STN Seminar Schedule - N. America
NEWS	2	"Ask CAS" for self-help around the clock
NEWS	3 FEB 28	PATDPAFULL - New display fields provide for legal status data from INPADOC
NEWS	4 FEB 28	BABS - Current-awareness alerts (SDIs) available
NEWS	5 MAR 02	GBFULL: New full-text patent database on STN
NEWS	6 MAR 03	REGISTRY/ZREGISTRY - Sequence annotations enhanced
NEWS	7 MAR 03	MEDLINE file segment of TOXCENTER reloaded
NEWS	8 MAR 22	KOREAPAT now updated monthly; patent information enhanced
NEWS	9 MAR 22	Original IDE display format returns to REGISTRY/ZREGISTRY
NEWS	10 MAR 22	PATDPASPC - New patent database available
NEWS	11 MAR 22	REGISTRY/ZREGISTRY enhanced with experimental property tags
NEWS	12 APR 04	EPFULL enhanced with additional patent information and new fields
NEWS	13 APR 04	EMBASE - Database reloaded and enhanced
NEWS	14 APR 18	New CAS Information Use Policies available online
NEWS	15 APR 25	Patent searching, including current-awareness alerts (SDIs), based on application date in CA/CAPLUS and USPATFULL/USPAT2 may be affected by a change in filing date for U.S. applications.
NEWS	16 APR 28	Improved searching of U.S. Patent Classifications for U.S. patent records in CA/CAPLUS
NEWS	17 MAY 23	GBFULL enhanced with patent drawing images
NEWS	18 MAY 23	REGISTRY has been enhanced with source information from CHEMCATS
NEWS	19 JUN 06	The Analysis Edition of STN Express with Discover! (Version 8.0 for Windows) now available
NEWS	20 JUN 13	RUSSIAPAT: New full-text patent database on STN
NEWS	21 JUN 13	FRFULL enhanced with patent drawing images
NEWS	22 JUN 27	MARPAT displays enhanced with expanded G-group definitions and text labels
NEWS	23 JUL 01	MEDICONF removed from STN
NEWS	24 JUL 07	STN Patent Forums to be held in July 2005
NEWS	25 JUL 13	SCISEARCH reloaded
NEWS	26 JUL 20	Powerful new interactive analysis and visualization software, STN AnaVist, now available
NEWS EXPRESS	JUNE 13	CURRENT WINDOWS VERSION IS V8.0, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 13 JUNE 2005
NEWS HOURS		STN Operating Hours Plus Help Desk Availability
NEWS INTER		General Internet Information
NEWS LOGIN		Welcome Banner and News Items
NEWS PHONE		Direct Dial and Telecommunication Network Access to STN

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NEWS WWW CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that specific topic.

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* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 11:47:31 ON 03 AUG 2005

=> file reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.21

0.21

FILE 'REGISTRY' ENTERED AT 11:47:36 ON 03 AUG 2005

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 2 AUG 2005 HIGHEST RN 857941-82-3

DICTIONARY FILE UPDATES: 2 AUG 2005 HIGHEST RN 857941-82-3

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

Please note that search-term pricing does apply when conducting SmartSELECT searches.

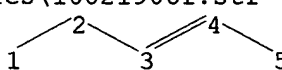
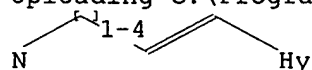
*
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added, *
* effective March 20, 2005. A new display format, IDERL, is now *
* available and contains the CA role and document type information. *
*

Structure search iteration limits have been increased. See HELP SLIMITS for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10821906f.str



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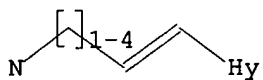
chain nodes :
1 2 3 4 5
chain bonds :
1-2 2-3 3-4 4-5
exact/norm bonds :
1-2 4-5
exact bonds :
2-3 3-4

G1:C,O

Match level :
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:Atom

L1 STRUCTURE UPLOADED

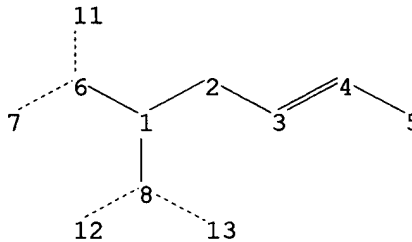
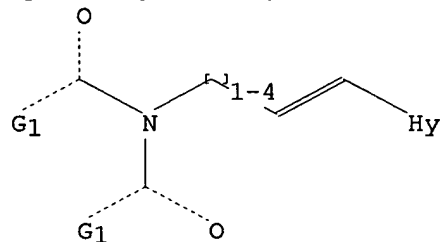
=> d l1
L1 HAS NO ANSWERS
L1 STR



G1 C,O

Structure attributes must be viewed using STN Express query preparation.

=>
Uploading C:\Program Files\Stnexp\Queries\10821906b.str



chain nodes :
1 2 3 4 5 6 7 8 11 12 13
chain bonds :
1-2 1-6 1-8 2-3 3-4 4-5 6-7 6-11 8-12 8-13
exact/norm bonds :
1-2 1-6 1-8 4-5 6-7 6-11 8-12 8-13
exact bonds :
2-3 3-4

G1:C,O

Match level :
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:Atom 6:CLASS 7:CLASS 8:CLASS 11:CLASS
12:CLASS 13:CLASS

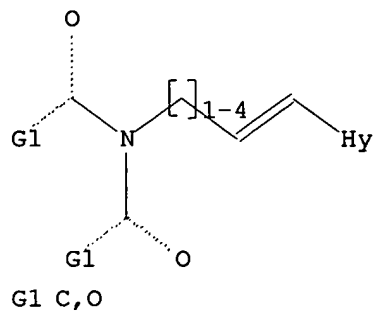
10/ 821,906

L2 STRUCTURE UPLOADED

=> d 12

L2 HAS NO ANSWERS

L2 STR



Structure attributes must be viewed using STN Express query preparation.

=>

Uploading C:\Program Files\Stnexp\Queries\10821906c.str



chain nodes :

1 2 3 4 5

chain bonds :

1-2 2-3 3-4 4-5

exact/norm bonds :

1-2 4-5

exact bonds :

2-3 3-4

G1:C,O

Match level :

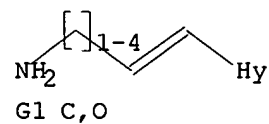
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:Atom

L3 STRUCTURE UPLOADED

=> d 13

L3 HAS NO ANSWERS

L3 STR

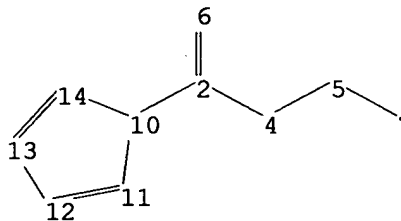
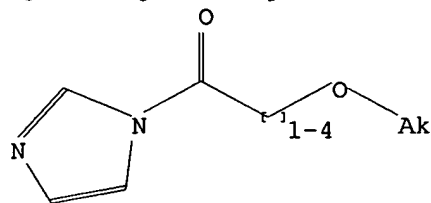


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Structure attributes must be viewed using STN Express query preparation.

=>

Uploading C:\Program Files\Stnexp\Queries\10821906e.str



chain nodes :

2 4 5 6 7

ring nodes :

10 11 12 13 14

chain bonds :

2-6 2-4 2-10 4-5 5-7

ring bonds :

10-11 10-14 11-12 12-13 13-14

exact/norm bonds :

2-6 2-10 4-5 5-7 10-11 10-14 12-13 13-14

exact bonds :

2-4 11-12

isolated ring systems :

containing 10 :

G1:C,O

Match level :

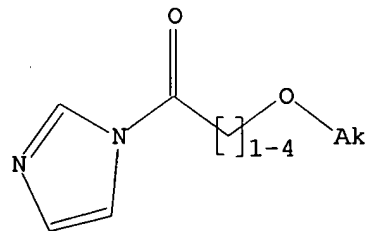
2:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 10:Atom 11:Atom 12:Atom 13:Atom
14:CLASS

L4 STRUCTURE UPLOADED

=> d 14

L4 HAS NO ANSWERS

L4 STR



G1 C,O

Structure attributes must be viewed using STN Express query preparation.

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=> d his

(FILE 'HOME' ENTERED AT 11:47:31 ON 03 AUG 2005)

FILE 'REGISTRY' ENTERED AT 11:47:36 ON 03 AUG 2005

L1 STRUCTURE UPLOADED
L2 STRUCTURE UPLOADED
L3 STRUCTURE UPLOADED
L4 STRUCTURE UPLOADED

=> s 11 sample

SAMPLE SEARCH INITIATED 11:49:47 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 61199 TO ITERATE

3.3% PROCESSED 2000 ITERATIONS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

50 ANSWERS

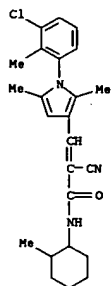
FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
 BATCH **COMPLETE**
PROJECTED ITERATIONS: EXCEEDS 1000000
PROJECTED ANSWERS: EXCEEDS 47773

L5 50 SEA SSS SAM L1

=> d scan 15

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LS 50 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN
IN 2-Propenamide, 3-[1-(3-chloro-2-methylphenyl)-2,5-dimethyl-1H-pyrrol-3-yl]-
2-cyano-N-(2-methylcyclohexyl)- (9CI)
MF C24 H28 Cl N3 O



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

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=> s l1 full

FULL SEARCH INITIATED 11:50:36 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - >1,000,000 TO ITERATE

< 80.7% PROCESSED 992034 ITERATIONS

41622 ANSWERS

< 81.4% PROCESSED 1000000 ITERATIONS

41960 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.17

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: EXCEEDS 1000000

PROJECTED ANSWERS: EXCEEDS 50885

L6 41960 SEA SSS FUL L1

=> d his

(FILE 'HOME' ENTERED AT 11:47:31 ON 03 AUG 2005)

FILE 'REGISTRY' ENTERED AT 11:47:36 ON 03 AUG 2005

L1 STRUCTURE UPLOADED

L2 STRUCTURE UPLOADED

L3 STRUCTURE UPLOADED

L4 STRUCTURE UPLOADED

L5 50 S L1 SAMPLE

L6 41960 S L1 FULL

=> s l2 sub=l1

L1 MAY NOT BE USED HERE

The L-number must have been created by a search in this file. To see all L-numbers defined in this session, enter DISPLAY HISTORY at an arrow prompt (=>). For additional information on subset searching in this file, enter HELP SUBSET.

ENTER SUBSET L# OR (END):.

SEARCH ENDED BY USER

=> s l2 sub=l6 ful

FULL SUBSET SEARCH INITIATED 11:51:41 FILE 'REGISTRY'

FULL SUBSET SCREEN SEARCH COMPLETED - 63 TO ITERATE

100.0% PROCESSED 63 ITERATIONS

10 ANSWERS

SEARCH TIME: 00.00.01

L7 10 SEA SUB=L6 SSS FUL L2

=> s l3 sub=l6 ful

FULL SUBSET SEARCH INITIATED 11:52:01 FILE 'REGISTRY'

FULL SUBSET SCREEN SEARCH COMPLETED - 41960 TO ITERATE

100.0% PROCESSED 41960 ITERATIONS

2481 ANSWERS

SEARCH TIME: 00.00.01

L8 2481 SEA SUB=L6 SSS FUL L3

=> s l4 sub=l6 ful

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FULL SUBSET SEARCH INITIATED 11:52:28 FILE 'REGISTRY'
FULL SUBSET SCREEN SEARCH COMPLETED - 0 TO ITERATE

100.0% PROCESSED 0 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

L9 0 SEA SUB=L6 SSS FUL L4

=> file casreact

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	278.92	279.13

FILE 'CASREACT' ENTERED AT 11:52:42 ON 03 AUG 2005
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FILE CONTENT:1840 - 31 Jul 2005 VOL 143 ISS 5

New CAS Information Use Policies, enter HELP USAGETERMS for details.

* CASREACT now has more than 9.2 million reactions *
* *****

Some CASREACT records are derived from the ZIC/VINITI database (1974-1991) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d his

(FILE 'HOME' ENTERED AT 11:47:31 ON 03 AUG 2005)

FILE 'REGISTRY' ENTERED AT 11:47:36 ON 03 AUG 2005

L1 STRUCTURE UPLOADED
L2 STRUCTURE UPLOADED
L3 STRUCTURE UPLOADED
L4 STRUCTURE UPLOADED
L5 50 S L1 SAMPLE
L6 41960 S L1 FULL
L7 10 S L2 FUL SUB=L6
L8 2481 S L3 FUL SUB=L6
L9 0 S L4 FUL SUB=L6

FILE 'CASREACT' ENTERED AT 11:52:42 ON 03 AUG 2005

=> s 17 or 18

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1 L7
205 L8
L10 205 L7 OR L8

=> s l10 and (deprotect? or hydroly? or cleav?)

13031 DEPROTECT?

63891 HYDROLY?

41189 CLEAV?

L11 41 L10 AND (DEPROTECT? OR HYDROLY? OR CLEAV?)

=> s l10 and ((acid chloride) or (acid imidazol?)).

173224 ACID

92027 CHLORIDE

5937 ACID CHLORIDE

(ACID(W) CHLORIDE)

173224 ACID

13008 IMIDAZOL?

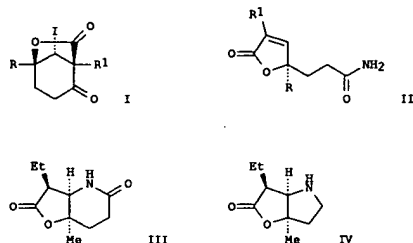
112 ACID IMIDAZOL?

(ACID(W) IMIDAZOL?)

L12 3 L10 AND ((ACID CHLORIDE) OR (ACID IMIDAZOL?))

L11 ANSWER 1 OF 41 CASREACT COPYRIGHT 2005 ACS on STN

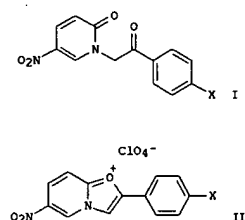
ACCESSION NUMBER: 142:134394 CASREACT
 TITLE: Ammonia-Promoted Fragmentation of 2-Alkyl- and 2,4-Dialkyl-3-iodo-1-oxocyclohexan-2,4-carbolactones
 AUTHOR(S): Dai, Mingshi; Zhang, Xuqing; Khim, Seock-Kyu; Schultz, Arthur G.
 CORPORATE SOURCE: Department of Chemistry, Rensselaer Polytechnic Institute, Troy, NY, 12180, USA
 SOURCE: Journal of Organic Chemistry (2005), 70(1), 384-387
 CODEN: JOCEAH; ISSN: 0022-3263
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



AB Nonracemic alkyl- and dialkylidioxabicyclooctanediones I undergo ammonia-promoted fragmentation to yield nonracemic aminooxopropyl butenolides II as the major products in most cases; γ -butyrolactones, and β,γ -epoxycyclohexanones are also formed in some cases. The product distribution of the fragmentation reaction is governed by the relative size of the substituents at C-2 and C-4 of the cyclohexanones; when the bridgehead substituent next to the oxygen of the bridge is large, regioselective addition of ammonia leads to the aminooxopropyl butenolide II as the major product, while smaller substituents lead to addition of ammonia to both the ketone and lactone carbonyl groups. II (R = Me; R1 = Et) is converted stereoselectively to the hexahydrofuro[2,3-b]pyridinedione III by treatment with cesium fluoride and tetra-Et silicate in methylene chloride; II (R = B) do not undergo the cyclization reaction. II (R = Me; R1 = Et) is also converted to the tetrahydrofuro[2,3-b]pyridone IV in two or three steps; oxidative Hofmann rearrangement of II followed either by treatment with cesium fluoride and tetra-Et silicate and acid-mediated deprotection or by acid-mediated cyclization and deprotection yields IV stereoselectively. Products such as IV may be useful in the synthesis of

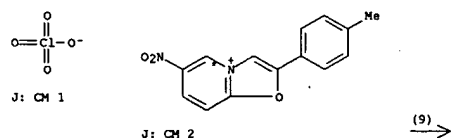
L11 ANSWER 2 OF 41 CASREACT COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 140:321266 CASREACT
 TITLE: Synthesis of 6-nitroderivatives of oxazolo[3,2-a]pyridines and their reactions with nucleophiles
 AUTHOR(S): Bush, Alexander A.; Babaev, Eugene V.
 CORPORATE SOURCE: Chemistry Department, Moscow State University, Moscow, 119899, Russia
 SOURCE: Molecules (2003), 8(6), 460-466
 CODEN: MOLEFW; ISSN: 1420-3049
 URL: <http://www.mdpi.org/molecules/papers/80600460.pdf>
 PUBLISHER: Molecular Diversity Preservation International
 DOCUMENT TYPE: Journal; (online computer file)
 LANGUAGE: English
 GI



AB 5-Nitro-2-pyridone can be selectively N-phenacylated, and the resulting phenacylpyridones I undergo cyclization to 6-nitrooxazolo[3,2-a]pyridinium salts II. II readily react with ammonia and aliphatic amines leading to the products of pyridine ring opening - previously unknown 1-amino-2-nitro-4-(oxazole-2-yl)buta-1,3-dienes. Reaction of II with water lead to hydrolytic cleavage of the oxazole fragment.

RX(9) OF 24 ...J ==> U

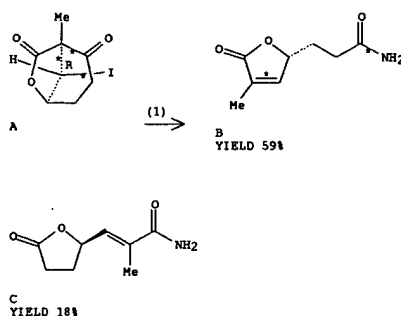


L11 ANSWER 1 OF 41 CASREACT COPYRIGHT 2005 ACS on STN

(Continued)

pyrrolizine alkaloids.

RX(1) OF 23 A ==> B + C

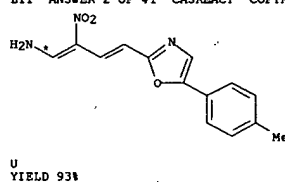


RX(1) RCT A 210684-51-8
 RGT D 7664-41-7 NH3
 PRO B 825653-24-5, C 825653-31-4
 SOL 109-99-9 THF
 NTE chemoselective
 REFERENCE COUNT: 32

THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 2 OF 41 CASREACT COPYRIGHT 2005 ACS on STN

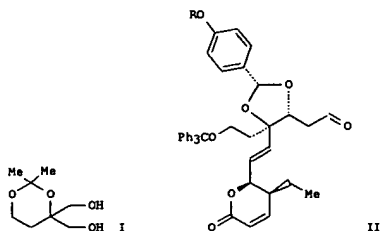
(Continued)



RX(9) RCT J 679407-23-9
 RGT V 7664-41-7 NH3
 PRO U 679407-30-8
 SOL 68-12-2 DMF

THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

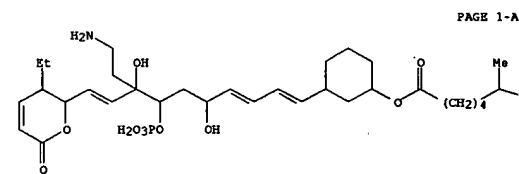
L11 ANSWER 3 OF 41 CASREACT COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 138:368651 CASREACT
 TITLE: Total Synthesis of Leustroducsin B
 AUTHOR(S): Shimada, Kousei; Kaburagi, Yosuke; Fukuyama, Tohru
 CORPORATE SOURCE: Graduate School of Pharmaceutical Sciences, The University of Tokyo, Bunkyo, Tokyo, 113-0033, Japan
 SOURCE: Journal of the American Chemical Society (2003), 125(14), 4048-4049
 CODEN: JACSAT; ISSN: 0002-7863
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



AB A convergent total synthesis of leustroducsin B, which is known to exhibit a variety of biol. activities, was successfully carried out. Notable features of the synthesis include construction of the C8 stereocenter by lipase-mediated desymmetrization of meso-diol I (90.2% ee) and preparation of the C9-C11 anti-diol moiety by the addition of an alkynylzinc reagent to the aldehyde II (R = SiMe₂CHMe₃). Furthermore, a new diol protecting group, p-silyloxybenzylidene, was developed for the deprotection from densely functionalized substrates under weakly acidic conditions. The protecting group was easily removed in a two-step procedure ((HF)·3·Et₃N; AcOH-THF-H₂O).

RX(35) OF 741 ...BZ ==> DJ

L11 ANSWER 3 OF 41 CASREACT COPYRIGHT 2005 ACS on STN (Continued)



PAGE 1-A

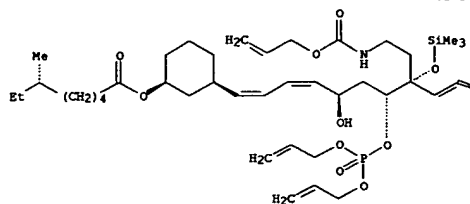
PAGE 1-B

Et
 DJ
 YIELD 51%

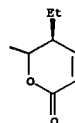
RX(35) RCT BZ 521274-48-6
 RGT DK 64-18-6 HCO₂H, L 121-44-8 Et₃N
 PRO DJ 145142-02-1
 CAT 14221-01-3 Pd(PPh₃)₄
 SOL 109-99-9 THF
 REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 3 OF 41 CASREACT COPYRIGHT 2005 ACS on STN (Continued)

PAGE 1-A



PAGE 1-B

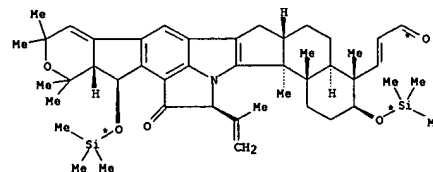


BZ

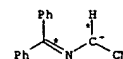
(35)

L11 ANSWER 4 OF 41 CASREACT COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 138:238323 CASREACT
 TITLE: Nodulisporic acid side-chain modifications: access to the 2'', 3'', 4'', and 6'' registers
 AUTHOR(S): Chakravarty, Prasun K.; Shih, Thomas L.; Colletti, Steven L.; Ayer, Michelle B.; Snedden, Christine; Kuo, Howard; Tyagarajan, Sricam; Gregory, Lynn; Zakson-Alken, Michelle; Shoop, Wesley L.; Schmatz, Dennis M.; Wyvratt, Matthew J.; Fisher, Michael H.; Meinke, Peter T.
 CORPORATE SOURCE: Merck Research Laboratories, Rahway, NJ, 07065-0900, USA
 SOURCE: Bioorganic & Medicinal Chemistry Letters (2003), 13(1), 147-150
 CODEN: BMCLE8; ISSN: 0960-894X
 PUBLISHER: Elsevier Science Ltd.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Efficient routes to access the 2'', 3'', 4'', and 6'' registers of the nodulisporic acid (NsA) side chain are disclosed. A mild one-carbon, PhZC≡NCH₂C(=O)Ph mediated homologation of NsA's 3''-aldehyde permitted access to the 4''-register. Curtius reaction of NsA's 3''-acid yielded the corresponding 2''-aldehyde from which the unnatural Δ²,3''-olefin isomers were obtained. In addition, Arndt-Eistert reactions of the parent NsA permitted a one-carbon homologation to the 6'' register. These efforts identified new analogs with significant flea activity and illustrated the biol. significance of unsatn. at the 1'', 2'' register.

RX(3) OF 210 ...C + I ==> J...



C



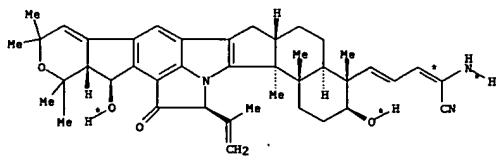
• Li⁺

I

(3)

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L11 ANSWER 4 OF 41 CASREACT COPYRIGHT 2005 ACS on STN (Continued)

J
YIELD 65%

RX(3) RCT C 412280-13-0, I 133618-69-6

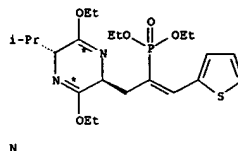
STAGE(1)
SOL 109-99-9 THFSTAGE(2)
PRO J 502179-87-5
NTE hydrolysis second stage
REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 5 OF 41 CASREACT COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 137:370155 CASREACT
 TITLE: Diastereoselective synthesis of 4-alkylidene-2-amino-4-phosphonobutanoic acids
 AUTHOR(S): Fernandez, M. Carmen; Ruiz, Maria; Ojea, Vicente; Quintela, Jose M.
 CORPORATE SOURCE: Departamento de Química Fundamental, Universidade da Coruña, Coruña, 15071 A, Spain
 SOURCE: Tetrahedron Letters (2002), 43(34), 5909-5912
 CODEN: TETLEY; ISSN: 0040-4039
 PUBLISHER: Elsevier Science Ltd.
 DOCUMENT TYPE: Journal
 LANGUAGE: English

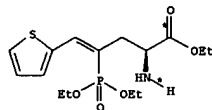
AB Olefination of Li derivs. of (2R,5S)-3,6-diethoxy-2,5-dihydro-2-isopropyl-5-(2-R-2-diethoxyphosphinylethyl)pyrazine (4b, R = SiMe₃; 4c, R = PO₃(OEt)₂; 4d, R = SnPh₃) with benzaldehyde affords (Z)- and (E)-isomers of corresponding 5-(2-(R1-methylidene)-2-diethoxyphosphinylethyl)pyrazine derivs. 7A and 8A (R1 = Ph), resp. The olefination of Li-4d- by R1CHO proceeds stereoselectively, giving only (Z)-isomers 7A-7E (R1 = Ph, A; Me₂CH, B; 2-thienyl, C; PhCH₂CH₂, D). The same reaction of 4d with cyclohexanone gave 2'-cyclohexylidene derivative 7E. The transition state and intermediate adduct for (Z)-isomer formation are preferred over (E)-isomer structures by 2.3 and 3.6 kcal/mol, resp., according to semi-empirical MO calcs. with PM3 Hamiltonian. Mild acid hydrolysis of 7A-C and 8A gave Et (Z)-(2S)-2-amino-4-diethoxyphosphinyl-4-(R1-methylidene)butanoates 10A-C and (E)-isomer 11A. Free AP4 derivs.; (2S)-2-amino-4-phosphono-4-(R1-methylidene)butanoic acids (Z)-12A,B and (E)-13A were obtained by 12N HCl hydrolysis of corresponding esters with the same double bond geometry, while hydrolysis of (Z)-10C required a sequential treatment with Me₃SiBr and LiOH and gave the isomerized product (E)-13C (R1 the same for A-E throughout the text).

RX(10) OF 33 ...N ==> W...



N

L11 ANSWER 5 OF 41 CASREACT COPYRIGHT 2005 ACS on STN (Continued)

W
YIELD 90%RX(10) RCT N 475143-67-0
RGT T 7647-01-0 HCl
PRO W 475143-72-7
SOL 109-99-9 THF, 7732-18-5 Water
NTE stereoselectiveREFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

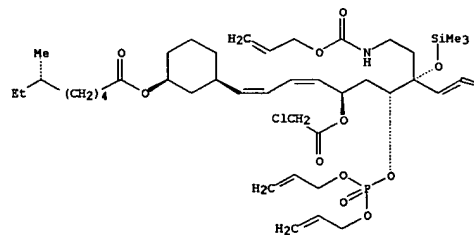
L11 ANSWER 6 OF 41 CASREACT COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 137:279001 CASREACT
 TITLE: Chemical transformation of Leustroduccins: synthesis of Leustroduccin B
 AUTHOR(S): Matsuhashi, Hayao; Shimada, Kousei
 CORPORATE SOURCE: Medicinal Chemistry Research Laboratories, Sankyo Co. Ltd, Shinagawa-ku, Tokyo, 140-8710, Japan
 SOURCE: Tetrahedron (2002), 58(28), 5619-5626
 CODEN: TETRAH; ISSN: 0040-4020
 PUBLISHER: Elsevier Science Ltd.
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB Chemical transformation of leustroduccin H to leustroduccin B was successfully accomplished in 11 steps including enzymic hydrolysis of phosphate ester. The process described here enables to differentiate all hydroxyl groups, amino and phosphate functionality so that this process would serve as a useful template for the preparation of whole different kinds of synthetic derivs. in structure activity relationship study. Absolute configuration of the side chain carboxylic acid has been determined as (S) configuration by Akasaka's method.

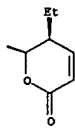
RX(1) OF 119 ...A ==> B...

PAGE 1-A



L11 ANSWER 6 OF 41 CASREACT COPYRIGHT 2005 ACS on STN (Continued)

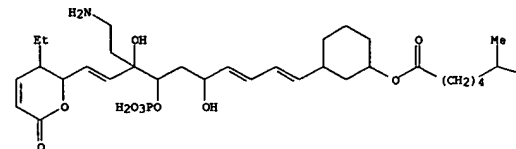
PAGE 1-B



A

(1) →

PAGE 1-A



PAGE 1-B

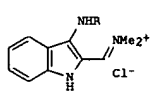
Et

B
YIELD 41%

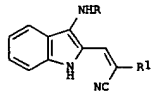
RX(1) RCT A 467234-69-1

STAGE(1)

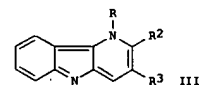
L11 ANSWER 7 OF 41 CASREACT COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 136:369572 CASREACT
 TITLE: Synthesis and some transformations of derivatives of pyrido[3,2-b]indole (8-carboline)
 AUTHOR(S): Ryabova, S. Yu.; Alekseeva, L. M.; Granik, V. G.
 CORPORATE SOURCE: State Scientific Center RF "NIOPIK", Moscow, 103787, Russia
 SOURCE: Chemistry of Heterocyclic Compounds (New York, NY, United States) (Translation of Khimiya Geterotsiklicheskikh Soedinenii) (2001), 37(8), 997-1004
 CODEN: CHOCAL; ISSN: 0009-3122
 PUBLISHER: Kluwer Academic/Consultants Bureau
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



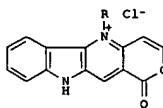
I



II



III



IV

AB Aminoindolemethaniminium chloride I (R = 4-O2NCGH4), prepared by the reaction of DMF and phosphoryl chloride with 3-(4-nitrophenylamino)indole, undergoes condensation reactions with compds. with acidic carbon-hydrogen bonds such as malononitrile and Et acetoacetate to give a variety of heterocyclic derivs., some containing the pyrido[3,2-b]indole (8-carboline) ring system. While condensation of either I or the corresponding aldehyde with cyanoacetamide or Et cyanoacetate gives the cyanovinylindoles II (R = 4-O2NCGH4; R1 = H2NCO, EtO2C), condensation of either Et acetoacetate or malononitrile with I gives the pyrido[3,2-b]indoles III (R = 4-O2NCGH4; R2 = H2N, Me; R3 = NC, EtO2C) or their hydrochlorides. Condensation of the aldehyde corresponding to I with Et acetoacetate gives various products depending on solvent and conditions. The hydrochloride of III (R = 4-O2NCGH4; R2 = Me; R3 = EtO2C) undergoes a condensation reaction with DMF di-Me acetal to give the aminovinyl pyrido[3,2-b]indole III (R = 4-O2NCGH4; R2 = Me2NCH:CH; R3 = EtO2C); hydrolysis of III (R = 4-O2NCGH4; R2 = Me2NCH:CH; R3 = EtO2C) with hydrochloric acid followed by cyclization gives the pyrano[3',4':5,6]pyrido[3,2-b]indolium chloride IV (R = 4-O2NCGH4).

RX(3) OF 26 ...C + I → J

L11 ANSWER 6 OF 41 CASREACT COPYRIGHT 2005 ACS on STN (Continued)

RGT C 1336-21-6 NH4OH
 SOL 67-56-1 MeOH, 7732-18-5 Water

STAGE(2)

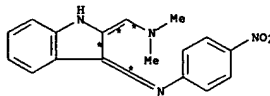
RGT D 64-18-6 HCO2H, E 121-44-8 Et3N
 CAT 14221-01-3 Pd(PPh3)4
 SOL 109-99-9 THF

PRO B 145142-82-1

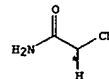
REFERENCE COUNT: 20

THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 7 OF 41 CASREACT COPYRIGHT 2005 ACS on STN (Continued)

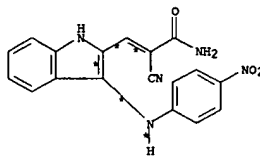


C



I

(3) →

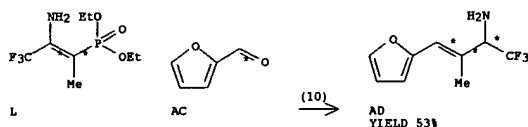
J
YIELD 92%

RX(3) RCT C 425368-78-1, I 107-91-5
 RGT G 121-44-8 Et3N
 PRO J 304465-27-8
 SOL 67-63-0 Me2CHOH

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 8 OF 41 CASREACT COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 136:294347 CASREACT
 TITLE: Fluoroalkyl α,β -Unsaturated Imines.
 Valuable Synthetic Intermediates from Primary
 Fluorinated Enamine Phosphonates
 AUTHOR(S): Palacios, Francisco; Pascual, Sergio; Oyarzabal,
 Julen; Ochoa de Retana, Ana M.
 CORPORATE SOURCE: Departamento de Química Orgánica I Facultad de
 Farmacia, Universidad del País Vasco, Vitoria, 01080,
 Spain
 SOURCE: Organic Letters (2002), 4(5), 769-772
 CODEN: ORLEF7; ISSN: 1523-7060
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB A simple method for the preparation of fluoroalkyl allyl amines or
 α,β -unsatd. ketones by an olefination reaction of primary
 enamine phosphonates and aldehydes, followed by selective reduction with
 hydrides or hydrolysis, is reported. Fluorinated β -amino
 nitriles are also obtained by an olefination reaction of primary enamine
 phosphonates with aldehydes and subsequent addition of metalated
 acetonitrile.

RX(10) OF 31 ...L + AC \longrightarrow AD

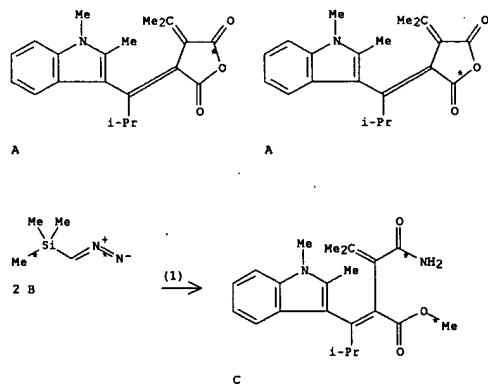


RX(10) RCT L 406951-60-8

STAGE(1)
 RGT Q 109-72-8 BuLi
 SOL 110-54-3 Hexane, 109-99-9 THF
 STAGE(2)
 RCT AC 98-01-1
 SOL 109-99-9 THF
 STAGE(3)
 RGT A 16940-66-2 NaBH4
 SOL 67-56-1 MeOH
 STAGE(4)
 RGT S 7647-01-0 HCl
 SOL 7732-18-5 Water
 STAGE(5)

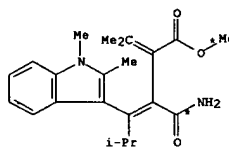
L11 ANSWER 9 OF 41 CASREACT COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 136:167056 CASREACT
 TITLE: Control of the association of indolylfulgimide with
 bis(acylamino)pyridine by photochromism
 AUTHOR(S): Okuyama, Tomyuki; Yokoyama, Yayoi; Yokoyama, Yasushi
 CORPORATE SOURCE: Department of Advanced Materials Chemistry, Graduate
 School of Engineering, Yokohama National University,
 Yokohama, 240-8501, Japan
 SOURCE: Bulletin of the Chemical Society of Japan (2001),
 74(11), 2181-2187
 CODEN: BCSJAB; ISSN: 0009-2673
 PUBLISHER: Chemical Society of Japan
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB While the association constant of the colored form (C) of a thermally
 irreversible photochromic indolylfulgimide with 2,6-
 bis(octanoylamino)pyridine in toluene at 21°C was 156 ± 11 mol-1
 dm3 through triplex hydrogen bonding, that of its colorless form (E),
 generated by visible-light irradiation, was increased to 885 ± 63 mol-1
 dm3. This result was supported by PM3 semiempirical mol.-orbital calcs.
 that the difference of the association consts. between the C-form and the
 E-form was mainly due to differences in the structures and conformations
 of the imide moiety.

RX(1) OF 8 2 A + 2 B \longrightarrow C + D...



L11 ANSWER 8 OF 41 CASREACT COPYRIGHT 2005 ACS on STN (Continued)
 RGT 7 1310-73-2 NaOH
 PRO AD 406951-66-4
 NTE stereoselective
 REFERENCE COUNT: 43 THERE ARE 43 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 9 OF 41 CASREACT COPYRIGHT 2005 ACS on STN (Continued)



D

RX(1) RCT A 145159-88-2

STAGE(1)
 RGT E 7664-41-7 NH3
 SOL 109-99-9 THF
 STAGE(2)
 RCT B 18107-18-1
 SOL 108-88-3 PhMe, 67-56-1 MeOH, 110-54-3 Hexane
 PRO C 396077-89-7, D 396077-90-0
 NTE 72% overall yield
 REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 10 OF 41 CASREACT COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 136:151166 CASREACT
 TITLE: Preparation of imidazoisoquinolinones as inhibitors of tyrosine kinases
 INVENTOR(S): Snow, Roger John; Cardozo, Mario; Goldberg, Daniel; Hammach, Abdelhakim; Morwick, Tina; Moss, Neil; Patel, Usha R.; Prokopowicz, Anthony S.; Takahashi, Hidenori; Tschantz, Matt Aaron; Wang, Xiao-Jun
 PATENT ASSIGNEE(S): Boehringer Ingelheim Pharmaceuticals, Inc., USA
 SOURCE: U.S. Pat. Appl. Publ., 62 pp., Cont.-in-part of U.S. Ser. No. 679,156.
 CODEN: USXXCO
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 2
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2002016460	A1	20020207	US 2001-921509	20010802
US 6506769	B2	20030114		
US 2003166929	A1	20030904	US 2002-292026	20021112
US 6770639	B2	20040803		

PRIORITY APPLN. INFO.:
 US 1999-157922P 19991006
 US 2000-679156 20001005
 US 2001-921509 20010802

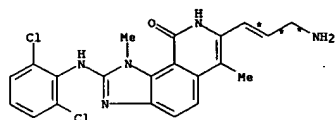
OTHER SOURCE(S): MARPAT 136:151166
 G1

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The title compds. [I: Ar1 = (un)substituted (non)aromatic carbocyclyl, heterocyclyl, heterocyclyl; X = NH, N(alkyl), O, etc.; Y = NR15, S, or Ra = H, alkyl, alkenyl, etc.; R4 and R5 together with the atom to which they are attached = II, III (wherein R6 = alkyl, H; R7 = alkyl, H; R8 = H, alkyl, etc.; R9 = H, CN, etc.)], useful as inhibitors of certain protein tyrosine kinases and are thus useful for treating diseases associated with such kinases, for example, diseases resulting from inappropriate cell proliferation, which include autoimmune diseases, chronic inflammatory diseases, allergic diseases, transplant rejection and cancer, as well as conditions resulting from cerebral ischemia, such as stroke, were prepared. All exemplified compds. I were evaluated in the tyrosine kinase assay using a kinase such as p56lck and were found to have IC50's less than 10 μ M. Methods of preparation are claimed and 29 example preps. are included.

E.g., a multi-step synthesis of the imidazoisoquinolinones IV was given. Claimed methods include: a method of making I wherein X is N-R15 and Ar1, R4, R5, R15 and Ra are as defined in Claim 1, said process comprising: (a) reacting a phenylenediamine with Ar1NCS in a suitable solvent at about ambient to reflux temperature for .apprx.3 to 24 h to provide a possibly substituted N-(o-aminophenyl)thiourea (b) reacting this product with a suitable activating agent chosen from 1,3-dicyclohexylcarbodiimide (DCC) and mercuric oxide in a suitable solvent at about ambient to reflux temperature

L11 ANSWER 10 OF 41 CASREACT COPYRIGHT 2005 ACS on STN (Continued)



CB
 YIELD 70%

RX (28)

STAGE(1)
 RGT BD 603-35-0 PPh3
 CAT 51364-51-3 Ph2-pentadienone Pd
 SOL 109-99-9 THF

STAGE(2)
 RCT BA 333455-34-8
 SOL 109-99-9 THF

STAGE(3)
 RGT CC 26628-22-8 NaN3
 SOL 7732-18-5 Water

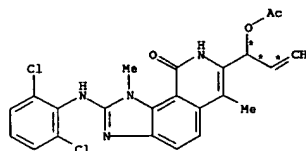
STAGE(4)
 RGT BD 603-35-0 PPh3

STAGE(5)
 RGT O 1336-21-6 NH4OH
 PRO CB 333455-47-3

L11 ANSWER 10 OF 41 CASREACT COPYRIGHT 2005 ACS on STN (Continued)

Also, a method of making I wherein X is S, Y is NH and Ar1, R4, R5 and Ra are as defined in claim 1, said process comprising: (a) reacting an aniline with Ar1NCS in a suitable solvent at about ambient to reflux temp. for .apprx.3 to 24 h to form a thiourea; (b) reacting this product under cyclizing conditions in a suitable solvent at about reflux temp. Also, a method of making V wherein R15, R8 and R9 are as described in claim 1, said method comprising: (a) reacting 2,6-dichloro-3-nitrobenzonitrile with NBR15 in a suitable solvent optionally in a pressure flask and at .apprx.0 to 80°, to provide 2-R15NH-3-nitro-6-chlorobenzonitriles, and subsequently reacting these compds. with ketoeater R9C(O)CH(R8)CO2Et in the presence of a suitable base in a suitable solvent, at about ambient temp. to form 2-NC-3-R15NH-4-O2NC6H2CR8 (C(O)R9)CO2Et (b) hydrolyzing this product by reacting with aq. acid, and cyclizing at about reflux temp., followed by reducing the cyclized product in a suitable solvent. Also, a method of making VI wherein Ra, R8, R9 and Ar1 are as described in claim 1, said method comprising: (a) reacting a phenylenediamine with Br2 in a suitable solvent at ambient temp. to provide a brominated ring product; (b) reacting this product with Ar1NCS in a suitable solvent at about ambient to reflux temp. for .apprx.3 to 24 h and subsequently reacting the product with a suitable activating agent chosen from DCC and mercuric oxide in a suitable solvent at about ambient to reflux temp. to form VI with Ra = Br; (c) cross-coupling to introduce Ra in place of Br in the presence of a suitable catalyst in a suitable solvent at .apprx.100°.

RX (28) OF 348 ...BA ==> CB...

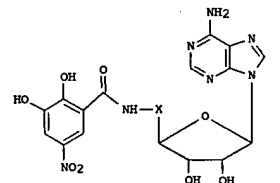


BA

(28)

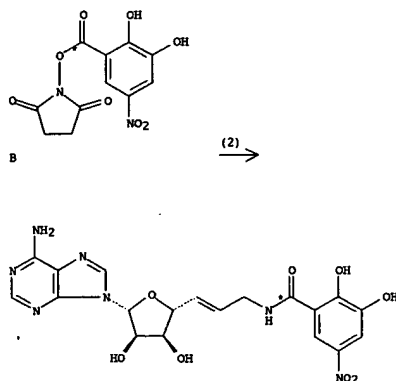
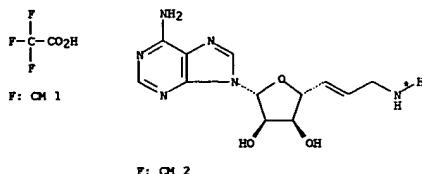
L11 ANSWER 11 OF 41 CASREACT COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 136:128144 CASREACT
 TITLE: X-ray crystal structure of a bisubstrate inhibitor bound to the enzyme catechol-O-methyltransferase: a dramatic effect of inhibitor preorganization on binding affinity
 AUTHOR(S): Lerner, Christian; Ruf, Armin; Gramlich, Volker; Masjost, Birgit; Zurcher, Gerhard; Jakob-Roetne, Roland; Borroni, Edilio; Diederich, Francois
 CORPORATE SOURCE: Laboratorium fur Organische Chemie, ETH-Zentrum, Zurich, 8092, Switz.
 SOURCE: Angewandte Chemie, International Edition (2001), 40(21), 4040-4042
 CODEN: ACIEF5; ISSN: 1433-7851
 PUBLISHER: Wiley-VCH Verlag GmbH
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 G1



AB Analogs of catechol-O-methyltransferase (COMT) bisubstrate inhibitor I: [X = -CH2CH2OCH2- (1)], with conformationally less flexible linkers, I [X = -(CH2)3- (2), -CH2CH=CH- (3)], are designed and prepared. In a radiochem. assay, compound 2 (IC50 199 nM) has a tenfold higher inhibitory potency than 1 (IC50 2 μ M). Compound 3 has an IC50 value of 9 nM, which is the most potent bisubstrate inhibitor for COMT to date. Thus, further rigidification of the spacer in I by introduction of a double bond has a tremendous effect on the binding affinity. An x-ray structure was determined at 2.6 Å resolution of the ternary complex formed from cocrystn. of 3, COMT, and Mg2+ ions. The inhibitor occupies, as predicted, both the SAM and catechol binding sites. The structure of the ternary complex closely resembles that known for the quaternary complex of COMT with S-adenosylmethionine (SAM), 3,5-dinitrocatechol, and a Mg2+ ion.

RX (2) OF 32 ...F + B ==> G



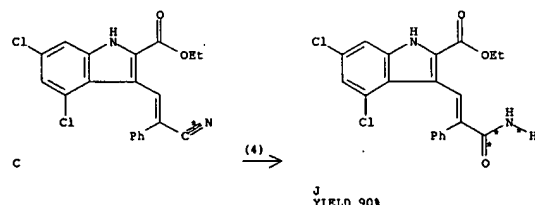
G
YIELD 80%

RX(2) RCT F 390381-61-0, B 273204-52-7
RGT D 121-44-8 Et3N
PRO G 390381-56-3
SOL 68-12-2 DMF

REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ACCESSION NUMBER: 134:326377 CASREACT
TITLE: Synthesis of (E)-3-(2-carboxy-2-pyridylvinyl)-4,6-dichloro-1H-indole-2-carboxylic acids, glycine-site NMDA receptor antagonists, utilizing the Knoevenagel condensation reaction
AUTHOR(S): Cregge, R. J.; Farr, R. A.; Friedrich, D.; Hulshof, J.; Janowick, D. A.; Meikrantz, S.; Metz, W. A.
CORPORATE SOURCE: Aventis Pharmaceuticals Inc., Bridgewater, NJ, 08807-0800, USA
SOURCE: Tetrahedron Letters (2001), 42(8), 1407-1409
CODEN: TETLEA; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The Knoevenagel condensation of arylacetonitriles with 4,6-dichloro-3-formyl-1H-indole-2-carboxylate, followed by hydrolysis, provides a convenient entry into a series of analogs of MDL 105,519, a selective glycine site N-methyl-D-aspartate (NMDA) receptor antagonist. Surprisingly, the hydrolysis of the indole arylpropenenitriles terminates at the formation of the corresponding carboxamide and does not proceed further to the desired dicarboxylic acid. However, when the aryl substituent is pyridine, hydrolysis proceeds via an azepinoindole unique to this series, which upon further hydrolysis converts smoothly to the desired dicarboxylic acid analog.

RX(4) OF 36 ...C ==> J...

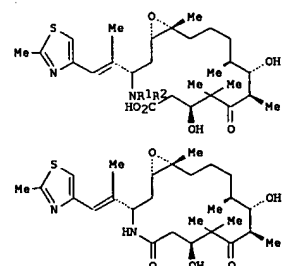


RX(4) RCT C 336783-62-1
RGT K 7664-93-9 H2SO4
PRO J 336783-65-4
SOL 64-19-7 AcOH

REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ACCESSION NUMBER: 131:31829 CASREACT
TITLE: A process for the preparation of ring-opened epothilone intermediates which are useful for the preparation of epothilone analogs
INVENTOR(S): Kim, Soong-Hoon; Borzilleri, Robert M.
PATENT ASSIGNEE(S): Bristol-Myers Squibb Company, USA
SOURCE: PCT Int. Appl., 20 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

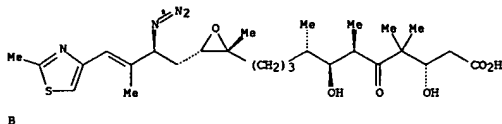
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9927890	A2	19990610	WO 1998-US25408	19981130
W:	AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GR, GM, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW, AM, AZ, BY, BG, BR, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
US 6365749	B1	20020402	US 1998-170582	19981013
CA 2312098	AA	19990610	CA 1998-2312098	19981130
EP 1035824	A1	20000920	EP 1998-960564	19981130
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI			
AU 739380	B2	20011011	AU 1999-16134	19981130
JP 2003522722	T2	20030729	JP 2000-522878	19981130
ZA 9810993	A	20000601	ZA 1998-10993	19981201
PRIORITY APPLN. INFO.:			US 1997-67550P	19971204
			WO 1998-US25408	19981130
OTHER SOURCE(S):			MARPAT 131:31829	
G1				



L11 ANSWER 13 OF 41 CASREACT COPYRIGHT 2005 ACS on STN (Continued)

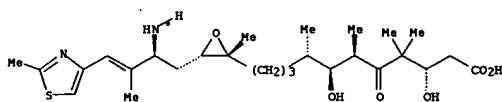
AB A process to produce ring opened epothilones (I) [NR1R2 = N3, (un)substituted amine] and their use in the preparation of epothilone analogs (II) is presented. Thus, epothilone B is cleaved with NaN3, azide reduced to amine and macrolactamized with diphenylphosphoryl azide to give II in 40% yield.

RX(2) OF 6 ...B ==> F...



B

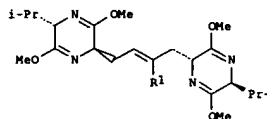
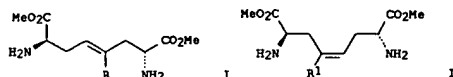
(2) →

F
YIELD 75%

RX(2) RCT B 219990-23-5
RGT G 1333-74-0 H2
PRO F 219990-28-7
CAT 1314-15-4 PtO2
SOL 64-17-5 EtOH

L11 ANSWER 14 OF 41 CASREACT COPYRIGHT 2005 ACS on STN

127:248372 CASREACT
TITLE: Stereoselective synthesis of alkenyl α,α'-bridged bis(glycines) using palladium promoted substitution in the bridge
AUTHOR(S): Efskind, Jon; Benneche, Tore; Undheim, Kjell
CORPORATE SOURCE: Dep. Chemistry, Univ. Oslo, Oslo, N-0315, Norway
SOURCE: Acta Chemica Scandinavica (1997), 51(9), 942-952
CODEN: ACHS7; ISSN: 0904-213X
PUBLISHER: Munksgaard
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

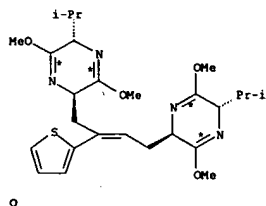


III

AB Conformationally constrained cystine analogs, I (R = H, Br, 2-thienyl, vinyl, β-styryl) and II (R1 = H, Br) have been synthesized which have an unsatd. four-carbon backbone-chain as a bridge between the α,α'-positions in two glycine units. The bridge was formed in a stereoselective dialkylation reaction between (E)- and (Z)-1,4-dibromo-2-butene or (E)- and (Z)-2-bromo-1,4-dihalogeno-2-butene and the chiral auxiliary (2S)-2,5-dihydro-3,6-dimethoxy-2-isopropylpyrazine to give (E)- and (Z)-bis(glycines) III (R1 = H, Br). Palladium mediated coupling between (E)- and (Z)-bis(glycines) III (R1 = Br) and Bu3SnR2 (R2 = 2-thienyl, vinyl, β-styryl, 2-phenylethynyl) provided for carbo-substitution at the olefinic carbon in the bridge. N-Methyl-2-pyrrolidinone was an excellent solvent for this reaction when triphenylarsine was the ligand for palladium. Mild hydrolytic conditions furnished the Me esters of the C4-bridged bis(glycine) derivs.

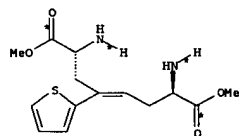
RX(6) OF 12 ...Q ==> W

L11 ANSWER 14 OF 41 CASREACT COPYRIGHT 2005 ACS on STN (Continued)



Q

(6) →

W
YIELD 77%

RX(6) RCT Q 195619-50-2
RGT W 7647-01-0 HCl
PRO W 195619-81-9
SOL 123-91-1 Dioxane, 7732-18-5 Water
REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

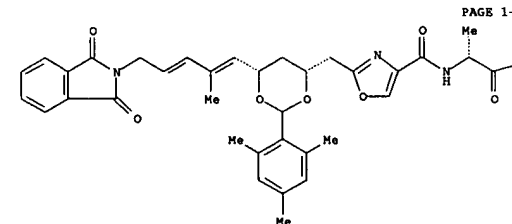
L11 ANSWER 15 OF 41 CASREACT COPYRIGHT 2005 ACS on STN

124:289061 CASREACT
TITLE: Total Synthesis of Streptogramin Antibiotics. (-)-Madumycin II
AUTHOR(S): Tavares, Francis; Lawson, Jon P.; Meyers, A. I.
CORPORATE SOURCE: Department of Chemistry, Colorado State University, Fort Collins, CO, 80523, USA
SOURCE: Journal of the American Chemical Society (1996), 118(13), 3303-4
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB A total synthesis of the title compound I (also called A-2315A) has been achieved for the first time in 29 steps and 1.8% overall yield. The sequence, utilizing chiral starting materials (S-malic acid and S-valinol) provided the correct chirality for the entire synthetic route. The synthetic plan was one of convergence wherein two key fragments, II and III, were coupled with each partner containing 2 and 3 stereogenic centers resp. The stereochem. of the C-13, C-15 hydroxyls was also confirmed as syn by two independent methods. A slight (8-10%) double bond isomerization in the diene moiety of synthetic I was found to be the result of the hydrolysis conditions to remove the dioxane in the penultimate product. This was verified by performing the hydrolysis on authentic madumycin II and observing the same small amount of diene isomer.

RX(17) OF 268 ...BH ==> BJ...

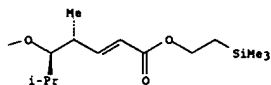


PAGE 1-A

10/ 821,906

L11 ANSWER 15 OF 41 CASREACT COPYRIGHT 2005 ACS on STN (Continued)

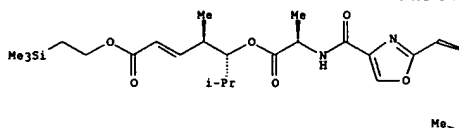
PAGE 1-B



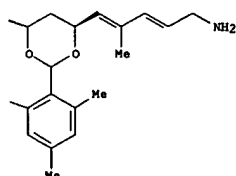
BH

(17)

PAGE 1-A



PAGE 1-B



BJ
YIELD 78%

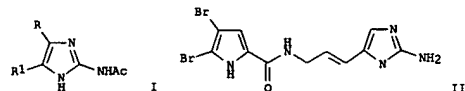
RX (17) RCT BH 175663-01-1
RGT BK 74-89-5 MeNH2

L11 ANSWER 15 OF 41 CASREACT COPYRIGHT 2005 ACS on STN (Continued)

PRO BJ 175663-02-2
SOL 64-17-5 EtOH, 71-43-2 Benzene

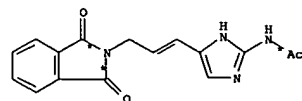
L11 ANSWER 16 OF 41 CASREACT COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 122:55805 CASREACT
TITLE: A Simple and Practical Synthesis of 2-Aminoimidazoles
AUTHOR(S): Little, Thomas L.; Webber, Stephen E.
CORPORATE SOURCE: Agouron Pharmaceuticals Inc., San Diego, CA, 92121, USA
SOURCE: Journal of Organic Chemistry (1994), 59(24), 7299-305
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

L11 ANSWER 16 OF 41 CASREACT COPYRIGHT 2005 ACS on STN (Continued)
RX(35) RCT BO 160072-69-5
RGT BB 302-01-2 N2H4
PRO BP 140381-63-3



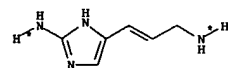
AB A new and simple two-step procedure to synthesize 2-aminoimidazoles (2-AI's) from readily available materials has been developed. The cyclization reaction of α -halo ketones RCOCH(R)X [$\text{R} = \text{Me}, \text{Et}, \text{CH}_2\text{Me}, \text{Ph}, 4\text{-BrC}_6\text{H}_4$, etc., $\text{R1} = \text{H}, \text{Me}, \text{Ph}, \text{R1} = (\text{CH}_2)_3, (\text{CH}_2)_4, \text{X} = \text{Cl}, \text{Br}$] and N -acetylguanidine in acetonitrile (MeCN) at reflux, or in DMF at ambient temperature, gives 4(5)-substituted and 4,5-disubstituted N -(1H-imidazol-2-yl)acetamides I, which are then hydrolyzed to their resp. 2-AI's. In general, the purified products were isolated in good yields. We have prepared several examples and have demonstrated the usefulness of this method by its application in the total synthesis of 2-aminohistamine, an interesting histamine analog, and oroidin (II), a marine natural product isolated from various sponges.

RX(35) OF 61 ...BO ==> BP...



BO

(35)



BP
YIELD 57%

L11 ANSWER 17 OF 41 CASREACT COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

118:191521 CASREACT

TITLE:

An efficient synthesis of substituted (Z)-allylamines and 7-membered nitrogen heterocycles from (Z)-3-(tributylstannyl)allylamine

AUTHOR(S):

Corriu, Robert J. P.; Geng, Bolin; Moreau, Joel J. E. Dep. Chim. Org. Fine, Univ. Montpellier II, Sci. Tech. Langue doc, Montpellier, F-34095, Fr.

SOURCE:

Journal of Organic Chemistry (1993), 58(6), 1443-8 CODEN: JOCEAH; ISSN: 0022-3263

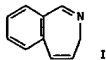
DOCUMENT TYPE:

Journal

LANGUAGE:

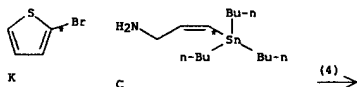
English

GI



AB The reaction of N-(trimethylsilyl)allylamine with 2 mol of n-butyllithium, followed by treatment with chlorotributyltin and subsequent hydrolysis, gave (Z)-3-(tributylstannyl)allylamine in high yields. The N,N-disilylated derivs., upon transmetalation of the C-Sn bond, led to unstable vinylolithium species. The latter readily underwent a [1,4] nitrogen to carbon silyl migration to give a lithium amide. The unprotected (Z)-3-(tributylstannyl)allylamine underwent a palladium-catalyzed cross-coupling reaction with aromatic bromides affording a stereospecific preparation of substituted allylic amines with Z configuration of the carbon-carbon double bond. The reactions of orthofunctionalized aryl bromides offer a one-step preparation of 7-membered nitrogen heterocycles, e.g. I, in high yields.

RX(4) OF 9 ...X + C ==> L

L
YIELD 70%

L11 ANSWER 18 OF 41 CASREACT COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

118:102293 CASREACT

TITLE:

Regio- and stereoselective synthesis of the tobacco alkaloid nicotine and its functionally substituted analogs

AUTHOR(S):

Rodinovskaya, L. A.; Bogomolova, O. P.; Shestopalov, A. M.; Litvinov, V. P. Inst. Org. Khim. im. Zelinskogo, Moscow, Russia

CORPORATE SOURCE:

Doklady Akademii Nauk (1992), 324(3), 585-8 [Chem.]

SOURCE:

CODEN: DAKNEQ; ISSN: 0869-5652

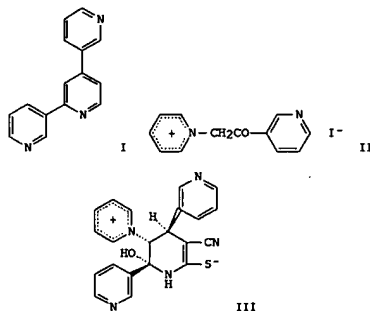
DOCUMENT TYPE:

Journal

LANGUAGE:

Russian

GI



AB The title compound I was regio- and stereoselectively synthesized in 4 steps starting from pyridinium salt II and RCH=C(CN)CSNH₂ (R = 2-pyridyl) to give the key intermediate pyridine derivative III.

RX(1) OF 10 A + B ==> C...

L11 ANSWER 17 OF 41 CASREACT COPYRIGHT 2005 ACS on STN

(Continued)

RX(4)

RCT X 1003-09-4, C 146829-37-0

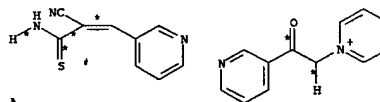
PRO L 146829-46-1

CAT 14221-01-3 Pd(PPh₃)₄

SOL 108-88-3 PhMe

L11 ANSWER 18 OF 41 CASREACT COPYRIGHT 2005 ACS on STN

(Continued)

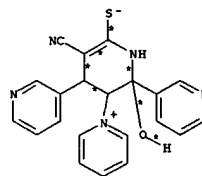


A

• I⁻

B

(1) →

C
YIELD 98%

RX(1)

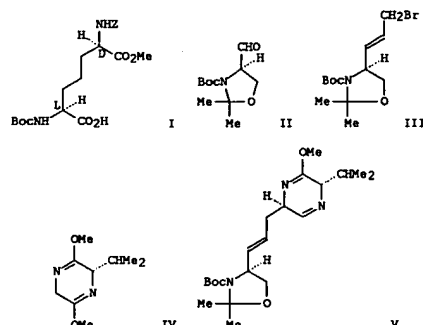
RCT A 132252-85-8, B 110514-05-1

PRO C 145917-22-2

SOL 64-17-5 EtOH

NTE regio- and stereoselective

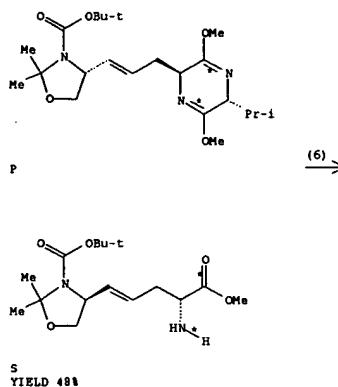
L11 ANSWER 19 OF 41 CASREACT COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 117:251724 CASREACT
 TITLE: Asymmetric synthesis of differentially protected meso-2,6-diaminopimelic acid
 AUTHOR(S): Jurgens, Alex R.
 CORPORATE SOURCE: Med. Res. Div., American Cyanamid Co., Pearl River, NY, 10965, USA
 SOURCE: Tetrahedron Letters (1992), 33(33), 4727-30
 CODEN: TELEAT; ISSN: 0040-4039
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



AB Differentially protected meso-2,6-diaminopimelic acid derivative I (Boc = Me₃CO₂C, Z = PhCH₂CO₂C) was prepared from D-serine-derived oxazolidine II. The key step was the stereoselective alkylation reaction of bromide III with dihydropyrazine IV in the presence of BuLi to give amino ester V.

RX(6) OF 45 ...P ==> B...

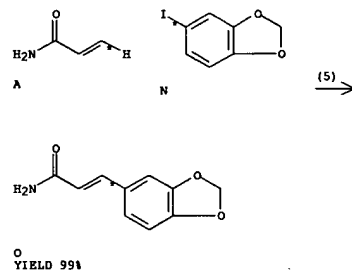
L11 ANSWER 19 OF 41 CASREACT COPYRIGHT 2005 ACS on STN (Continued)



RX(6) RCT P 142573-56-6
 RGT T 7647-01-0 HCl
 PRO S 144619-39-6
 SOL 109-99-9 THF, 7732-18-5 Water

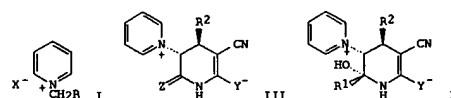
L11 ANSWER 20 OF 41 CASREACT COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 115:135611 CASREACT
 TITLE: A facile approach to arylacetaldehydes via polymeric palladium catalyst
 AUTHOR(S): Zhang, Zhuangyu; Pan, Yi; Hu, Hongwen; Kao, Tsiyu
 CORPORATE SOURCE: Dep. Chem., Nanjing Univ., Nanjing, 210008, Peop. Rep. China
 SOURCE: Synthesis (1991), (7), 539-42
 CODEN: SYNTHF; ISSN: 0039-7881
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Several arylacetaldehydes e.g., R₆H₄CH₂CHO (R = H, 2-, 4-Cl, 4-Br) were synthesized in moderate yields via Heck reaction of acrylamide with substituted iodobenzenes R₆CHI in the presence of a polymer-supported Pd catalyst, followed by Hofmann reaction and subsequent hydrolysis

RX(5) OF 20 A + N ==> O



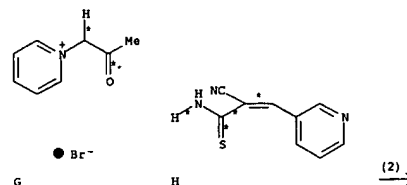
RX(5) RCT A 79-06-1, N 5876-51-7
 RGT D 127-09-3 AcONa
 PRO O 130873-12-5
 CAT 7440-05-3 Pd
 SOL 68-12-2 DMF, 7732-18-5 Water
 NTE Polymer-bound catalyst

L11 ANSWER 21 OF 41 CASREACT COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 114:101657 CASREACT
 TITLE: Stereoselective synthesis of 3,4-trans-1,2,3,4-tetrahydropyridines based on pyridinium ylides
 AUTHOR(S): Shestopalov, A. M.; Rodinovskaya, L. A.; Litvinov, V. P.; Sharanin, Yu. A.
 CORPORATE SOURCE: Inst. Org. Khim. im. Zelinskogo, Moscow, USSR
 SOURCE: Doklady Akademii Nauk SSSR (1990), 314(4), 870-5 [Chem.]
 CODEN: DANKAS; ISSN: 0002-3264
 DOCUMENT TYPE: Journal
 LANGUAGE: Russian
 GI

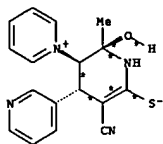


AB Treating alkylpyridinium halides I (R = CONH₂, X = Cl; R = CO₂Me, COR₁, R₁ = Ph, Me, X = Br; R = CS₂Me, cyclopropylcarbonyl, X = iodo) with Et₃N in EtOH gave the corresponding title ylides, which [R = CONH₂, CO₂Me] underwent cyclocondensation reaction with Z-R₂CH=C(CN)CO₂Et (R₂ = Ph) or Z-R₂CH=C(CN)CSNH₂ (II; R₂ = 4-FC₆H₄, 3-pyridyl) to give 3-tetrahydropyridinone inner salts III (Y, Z = O, S) regio- and stereoselectively in 54-82% yield. Analogous reaction of I (R = COR₁) with II gave 4-tetrahydropyridinols IV in 67-97% yield. III and IV were also prepared in 59-94% yield from I, R₂CHO, and NCCH₂R₃ (R₃ = CO₂Et, CSNH₂, C(NH₂):C(CN)₂). The IR and NMR spectra of III and IV were interpreted.

RX(2) OF 8 G + H ==> I



L11 ANSWER 21 OF 41 CASREACT COPYRIGHT 2005 ACS on STN (Continued)

I
YIELD 95%

RX(2) PCT G 17282-41-6, H 132252-85-8
 RGT E 121-44-8 Et3N
 PRO I 132252-90-5
 SOL 64-17-5 EtOH

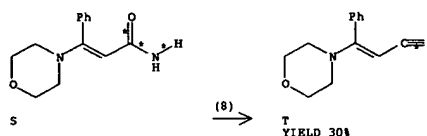
L11 ANSWER 22 OF 41 CASREACT COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 114:81537 CASREACT
 TITLE: Interaction of dichlorocarbene with substituted 3,4-dihydroisoquinolines and 1-methylene-1,2,3,4-tetrahydroisoquinolines
 AUTHOR(S): Khlebnikov, A. F.; Kostikov, R. R.; Shklyakov, V. S.; Aleksandrov, B. B.; Dormidontov, M. Yu.
 CORPORATE SOURCE: Leningr. Gos. Univ., Leningrad, 199004, USSR
 SOURCE: Khimiya Geterotsiklichesikh Soedinenii (1990), (8), 1086-91
 CODEN: KGSSAQ; ISSN: 0453-8234
 DOCUMENT TYPE: Journal
 LANGUAGE: Russian
 GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB :CCl2 added to dihydroisoquinolines I (R = H, R1 = R2 = Me; R = MeO, R1 = Et, R2 = Ph) to give 81-100% gem-dichloroazirino[2,1-a]isoquinolines II, which gave 49-61% benzazepinones III (X = Cl, OH, resp.) on hydrolysis and monochloro derivative IV on reduction with LiAlH4. Analogous reaction of I [R = H, R1 = Me, R2 = 2-(cyclohexylamino)ethyl] gave 30% II [R2 = 2-(N-cyclohexylformamido)ethyl], while tetrahydroisoquinoline deriva. V (R3 = OEt, NH2) gave 69% I (R = H, R1 = Me, R3 = CCl:CHCO2Et) and 50% spiroactam VI, resp. RX1 (X1 = NHCMe3, morpholino) added to PhC.tplbond.CCONH2 to give 45-73% PhCX1:CHCONH2, which reacted with :CCl2 to give 25% pyrrolinone VII and 30% E-PhCX1:CHCN (X1 = morpholino), resp.

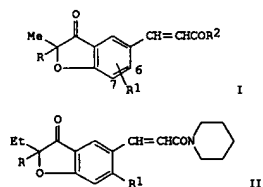
RX(8) OF 14 ...S ==> T



RX(8) RCT S 132067-92-6
 RGT D 1310-73-2 NaOH
 PRO T 119119-74-3
 CAT 56-37-1 PhCH2NMe3 Cl
 SOL 7732-18-5 Water, 67-66-3 CHCl3

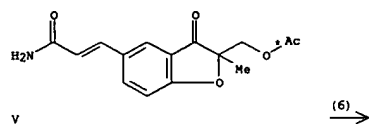
L11 ANSWER 23 OF 41 CASREACT COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 112:216589 CASREACT
 TITLE: Studies on the synthesis of antiulcer agents. VII. Synthesis and antiulcer activity of dihydrobenzofuranone derivatives
 AUTHOR(S): Kitazawa, Makio; Akahane, Masuo; Nakano, Yasushi; Hayakawa, Kazuhide; Sato, Kazuaki; Kobayashi, Michihiro
 CORPORATE SOURCE: Res. Lab., Kissei Pharm. Co., Ltd., Matsumoto, 399, Japan
 SOURCE: Yakugaku Zasshi (1989), 109(10), 737-48
 CODEN: YKKZAJ; ISSN: 0031-6903
 DOCUMENT TYPE: Journal
 LANGUAGE: Japanese
 GI

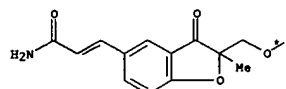


AB A number of 2-substituted (2,3-dihydro-3-oxo-5-benzofuryl)acrylates and -acrylamides I (R = H, HOCH2, AcOCH2, EtOCH2, NOCH2, etc.; R1 = H, 6-OMe, 7-OMe; R2 = OH, OEt, NH2, etc.) and II (R = HOCH2, AcOCH2; R1 = H, OMe) were prepared and tested for antiulcer activities to study structure-activity relationships. Significant antiulcer activities were found in I (R = HOCH2, AcOCH2; R1 = H, 6-OMe; R2 = piperidino, morpholino). Among the compds. tested, I (R = HOCH2, R1 = H, R2 = piperidino) was the most promising compound

RX(6) OF 184 ...V ==> W



L11 ANSWER 23 OF 41 CASREACT COPYRIGHT 2005 ACS on STN (Continued)

W
YIELD 81%

RX(6) RCT V 127006-61-5
 RGT H 1310-73-2 NaOH
 PRO W 127006-64-8
 SOL 64-17-5 EtOH, 7732-18-5 Water

L11 ANSWER 24 OF 41 CASREACT COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 112:76896 CASREACT

TITLE: Nitrile cyclization reactions. XXXIII. Synthesis and structure of 4-aryl-2,6-diamino-3,5-dicyanothiopyrans and their recyclization to 6-amino-4-aryl-3,5-dicyano-2(1H)-pyridinethiones

AUTHOR(S): Sharanin, Yu. A.; Shestopalov, A. M.; Nesterov, V. N.; Melenchuk, S. N.; Promonenkov, V. K.; Shklover, V. E.; Struchkov, Yu. T.; Litvinov, V. P.

CORPORATE SOURCE: Voroshilovgr. Gos. Pedagog. Inst., Voroshilovgrad, USSR

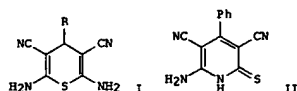
SOURCE: Zhurnal Organicheskoi Khimii (1989), 25(6), 1323-30

CODEN: ZORFAE; ISSN: 0514-7492

DOCUMENT TYPE: Journal

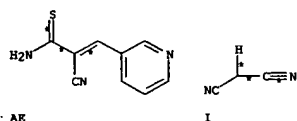
LANGUAGE: Russian

GI



AB Thiopyrans I (R = Ph, 4-FC₆H₄, 4-ClC₆H₄, 4-BrC₆H₄, 4-MeOC₆H₄, 3-pyridinyl, 4-piperidinyl) were prepared from NCCH₂CSNH₂ and RCH:C(CN)₂ from CH₂(CN)₂ and RCH:C(CN)CSNH₂, or from RCHO, CH₂(CN)₂, and NCCH₂CSNH₂. I (R = Ph) has a tub conformation based on x-ray crystal data; it rearranges to pyridinethione II via sequential treatment with morpholine and HCl.

RX(19) OF 33 AE + I ==> X



L11 ANSWER 25 OF 41 CASREACT COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 111:214846 CASREACT

TITLE: Glycosylaziridine derivatives

AUTHOR(S): Tronchet, Jean M. J.; Massoud, Mohamed A. M.

CORPORATE SOURCE: Inst. Pharm. Chem., Univ. Geneva, Geneva, 1211, Switz.

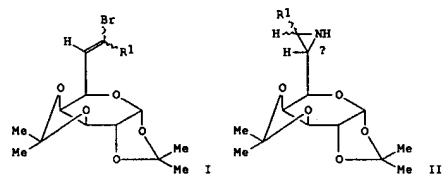
SOURCE: Heterocycles (1989), 29(3), 419-26

CODEN: HETCYM; ISSN: 0385-5414

DOCUMENT TYPE: Journal

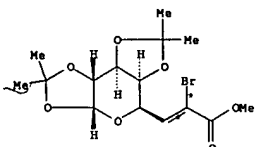
LANGUAGE: English

GI



AB Bromooctenopyranoses I (R₁ = cyano, COMe, C₆H₅, CO₂Me, CO₂Et) reacted with NH₃ in MeOH to give title aziridines II. In some reactions II were accompanied by I (R₁ = CONH₂) and II (R₁ = CONH₂).

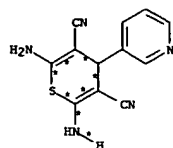
RX(4) OF 47 3 K ==> L + M + N...



2 K

L11 ANSWER 24 OF 41 CASREACT COPYRIGHT 2005 ACS on STN

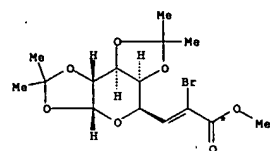
(Continued)

X
YIELD 90%

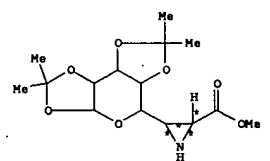
RX(19) RCT AE 109619-20-7, I 109-77-3
PRO X 125219-61-6
CAT 110-89-4 Piperidine
SOL 64-17-5 EtOH

L11 ANSWER 25 OF 41 CASREACT COPYRIGHT 2005 ACS on STN

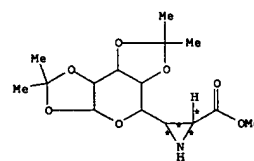
(Continued)



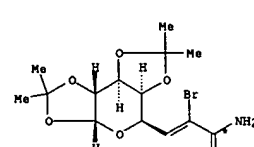
K



L



M



N

RX(4) RCT K 71553-97-4
RGT E 7664-41-7 NH₃
PRO L 81069-11-6, M 81069-15-0, N 123620-63-3
SOL 67-56-1 MeOH

L11 ANSWER 26 OF 41 CASREACT COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

TITLE:

AUTHOR(S):

CORPORATE SOURCE:

SOURCE:

DOCUMENT TYPE:

LANGUAGE:

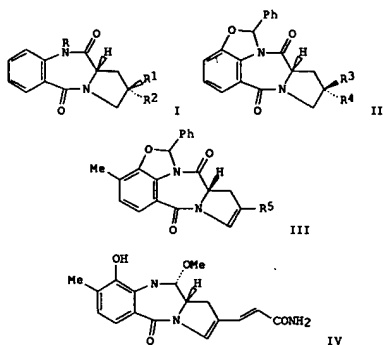
GI

111:96934 CASREACT

A total synthesis of anthramycin. Application of palladium-catalyzed coupling reactions for the attachment of the acrylic side chain

Pena, Michael R.; Stille, J. K.
Dep. Chem., Colorado State Univ., Fort Collins, CO,
80523, USAJournal of the American Chemical Society (1989),
111(14), 5417-24

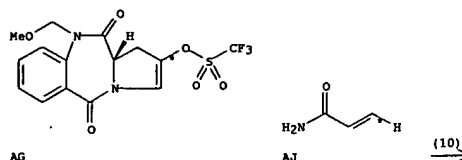
CODEN: JACSAT; ISSN: 0002-7863

Journal
English

AB Utilization of the Pd-catalyzed reactions of vinyl triflates obtained from model pyrrolobenzodiazepines I (R = Me, R1R2 = O; R = CH2OMe, CH2OEt, R1 = OH, R2 = H) either with β -(tributylstannyl)acrylates or acrylic esters and amides yields coupled products having the basic anthramycin framework. Generation of the enol triflates from the 2-keto precursors is regioselective, introducing the double bond in the pyrrole ring into the 2,3-position. Oxidation of the protected pyrrolobenzodiazepine II (R3 = OH, R4 = H) to III (R3R4 = O) followed by conversion to the vinyl triflate III (R5 = O3SCF3) provided the appropriate coupling partner for the attachment of the acrylamide side chain via a Pd-catalyzed reaction with acrylamide. Reduction of III [R = (E)-CH=CHCONH2] with NaBH4 and deprotection gave anthramycin Me ether IV. This sequence for the attachment of the

L11 ANSWER 26 OF 41 CASREACT COPYRIGHT 2005 ACS on STN (Continued)
acrylamide side chain provides a relatively short pathway to anthramycin and allows the facile synthesis of anthramycin analogs.

RX(10) OF 207 ...AG + AJ ==> AK

AK
YIELD 50%

RX(10) RCT AG 116642-18-3, AJ 79-06-1
RGT AL 280-57-9 Triethylenediamine
PRO AK 116642-20-7
CAT 14592-56-4 PdCl2(MeCN)2
SOL 67-56-1 MeOH

L11 ANSWER 27 OF 41 CASREACT COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

TITLE:

AUTHOR(S):

CORPORATE SOURCE:

SOURCE:

DOCUMENT TYPE:

LANGUAGE:

GI

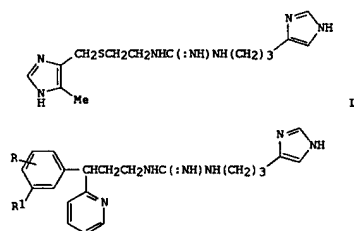
111:77913 CASREACT

Synthesis and in vitro pharmacology of apromidine and related phenyl(pyridylalkyl)guanidines, a potential new class of positive inotropic drugs

Buschauer, Armin
Inst. Pharm., Freie Univ. Berlin, Berlin, D-1000/33,
Fed. Rep. Ger.

Journal of Medicinal Chemistry (1989), 32(8), 1963-70

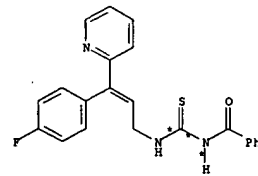
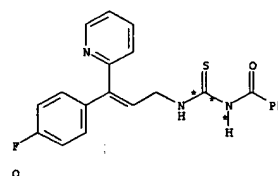
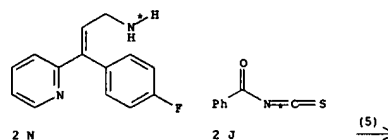
CODEN: JMCNAR; ISSN: 0022-2623

Journal
English

AB Replacement of the cimetidine moiety in apromidine (I) by more lipophilic H2-nonspecific pheniramine-like structures resulted in potent H2 agonists with up to 160 times the activity of histamine in the isolated, spontaneously beating guinea-pig right atrium. Also, these compds. proved to be moderate H1 antagonists. Highest H2-agonistic potency was found in compds. characterized by a three-membered carbon chain connecting the aromatic rings and the guanidine group. The activity in the atrium was increased 2-4-fold by halogen substituents in the meta or para position of the Ph ring. Highest H1-antagonistic potency resides in the group of para-halogenated compds., p-F representing the optimal substituent in both receptor models. Thus, guanidine II (R = 4-F, R1 = H) (apromidine) combines about 100 times the activity of histamine at the H2-receptor with H1-antagonistic potency in the range of pheniramine. Further increase in the activity on the atrium was achieved by disubstitution with halogen on the Ph ring, such as 3,4-F2, 3,5-F2, and 3,4-Cl2. The 2-pyridyl group in apromidine was replaced by 3-pyridyl without significant change in H2 agonistic activity, whereas the 4-pyridyl and Ph analogs were less active. The rank order of potency in the atrium was in good agreement with the pos. inotropic effects found in isolated perfused guinea pig hearts, where II (R = 4-F, R1 = F) R = 5-F; R1 = F; R = 4-Cl, R1 = Cl) were the most potent compds. as well.

RX(5) OF 152 2 N + 2 J ==> O + P...

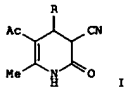
L11 ANSWER 27 OF 41 CASREACT COPYRIGHT 2005 ACS on STN (Continued)



RX(5) RCT N 121598-09-2, J 532-55-8
PRO O 121597-49-7, P 121598-19-4
SOL 67-66-3 CHCl3
NTE 80% Overall

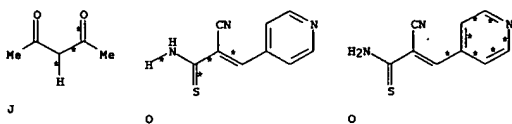
L11 ANSWER 28 OF 41 CASREACT COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 109:149305 CASREACT
 TITLE: 4-Substituted 4-dihydropyridine-2(3H)-thiones: synthesis, properties and cardiovascular activity
 AUTHOR(S): Krauze, A.; Vitolina, R.; Romanova, M. R.; Duburs, G.
 CORPORATE SOURCE: Inst. Org. Sint., Riga, USSR
 SOURCE: Khimiko-Farmatsevticheskii Zhurnal (1988), 22(5), 548-53
 CODEN: KHFZAN; ISSN: 0023-1134
 DOCUMENT TYPE: Journal
 LANGUAGE: Russian
 GI



AB 6-Methyl-5-acetyl-3-cyano-1,4-dihydropyridine-2(3H)-thiones I (R = Ph, p-O₂NC₆H₄, m-O₂NC₆H₄, p-ClC₆H₄, 4-pyridyl) and their water-soluble Na salts were prepared and their cardiovascular activity determined. ¹H-NMR shows that I (R = Ph, substituted Ph) are formed as cis and trans stereoisomers in 1.2:1.0 ratio. I (R = 4-pyridyl) exist as a betaine. The most pronounced and long-term vasodilator action on cardiac vessels and femoral artery is shown by I (R = m-O₂NC₆H₄, p-ClC₆H₄).

RX(7) OF 36 J + 2 O ==> P...

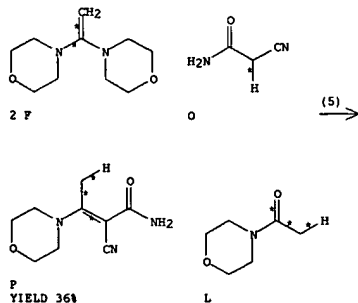


(7) →

L11 ANSWER 29 OF 41 CASREACT COPYRIGHT 2005 ACS on STN

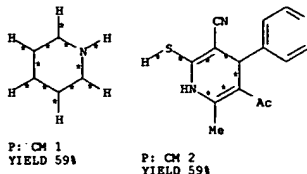
ACCESSION NUMBER: 107:236631 CASREACT
 TITLE: Condensation reactions of 1,1-dimorpholinoethene and of 1,1-dipiperidinoethene with carbon acids
 AUTHOR(S): Gandhi, Sham S.; Gibson, Martin S.
 CORPORATE SOURCE: Dep. Chem., Brock Univ., St. Catharines, ON, L2S 3A1, Can.
 SOURCE: Canadian Journal of Chemistry (1987), 65(12), 2717-21
 CODEN: CJCHAG; ISSN: 0008-4042
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB 1,1-Dimorpholinoethene and 1,1-dipiperidinoethene condense with carbon acids such as malononitrile, Et cyanoacetate, cyanoacetamide, and di-Et malonate to give the corresponding β,β-disubstituted enamine, with a mol. of morpholine or piperidine being eliminated in the process. Similar reactions with acetylacetone and Et acetoacetate proceed with loss of the acetyl group to give the β-substituted enamine. 1,1-Dipiperidinoethene and nitromethane give the β-nitroenamine. Secondary processes of either hydrolysis or further Michael addition and elimination are noted in condensations of 1,1-dimorpholinoethene or 1,1-dipiperidinoethene with cyanoacetamide under more basic conditions. 1,1-Dipiperidinoethene is arylated at the 2-position by 2,4-dinitrochlorobenzene.

RX(5) OF 16 2 F + O ==> P + L



RX(5) RCT F 14212-87-4, O 107-91-5
 PRO P 111505-56-7, L 1696-20-4
 NTE ether or THF solvent

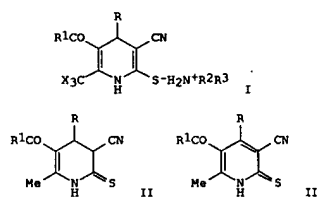
L11 ANSWER 28 OF 41 CASREACT COPYRIGHT 2005 ACS on STN (Continued)



RX(7) RCT J 123-54-6, O 109619-21-8
 RGT C 110-89-4 Piperidine
 PRO P 116736-43-7
 SOL 64-17-5 EtOH

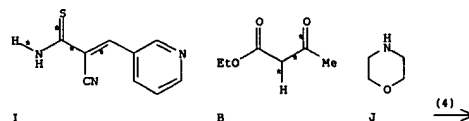
L11 ANSWER 30 OF 41 CASREACT COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 107:198023 CASREACT
 TITLE: Cyclization of nitriles. XXII. Reactions of arylideneacyanohydroacetamides with unsymmetric 1,5-dicarbonyl compounds. Molecular and crystal structure of 3-cyano-5-(ethoxycarbonyl)-4-(4-fluorophenyl)-6-methyl-2(1H)-pyridinethione
 AUTHOR(S): Sharanin, Yu. A.; Shestopalov, A. M.; Rodinovskaya, L. A.; Nesterov, V. N.; Shklover, V. E.; Struchkov, Yu. T.; Promonnikov, V. K.; Litvinov, V. P.
 CORPORATE SOURCE: Voroshilovgr. Gos. Pedagog. Inst., Voroshilovgrad, USSR
 SOURCE: Zhurnal Organicheskoi Khimii (1986), 22(12), 2600-9
 CODEN: ZORXAE; ISSN: 0514-7492
 DOCUMENT TYPE: Journal
 LANGUAGE: Russian
 GI

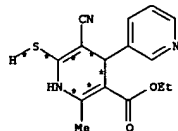


AB Pyridinecarboxitriles I (R = 2-furyl, 3-pyridyl, substituted Ph, R1 = EtO, Ph, R2 = R3 = Et, R2R3 = (CH₂)₅, (CH₂)₆, (CH₂)₂₀(CH₂)₂, X = H, F) were prepared in 28-81% yields by cyclocondensation of RCH:C(CN)CSNH₂ with CX₃COCH₂CO₂R1 and R2R3NH₂, with RCHO, CNCH₂CSNH₂, and CX₃COCH₂CO₂R1, and with RCH:C(CN)CSNH₂ and CX₃C(NR₂R3):CHCOR1. Hydrolysis of I by HCl gave nitrile II (R = p-ClC₆H₄, R1 = Ph) which was heated with concentrated HCl to give nitrile III. The crystal and mol. structure of III were confirmed by x-ray anal.

RX(4) OF 61 I + B + J ==> K



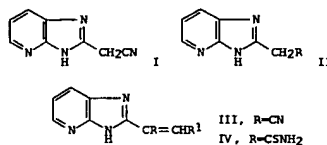
L11 ANSWER 30 OF 41 CASREACT COPYRIGHT 2005 ACS on STN (Continued)

K: CM 1
YIELD 71%K: CM 2
YIELD 71%

RX(4) RCT I 109619-20-7, B 141-97-9, J 110-91-8
PRO K 110951-24-1
SOL 64-17-5 EtOH

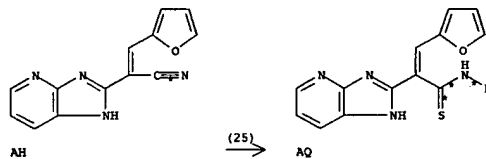
L11 ANSWER 31 OF 41 CASREACT COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 106:176258 CASREACT
TITLE: Synthesis and some reactions of 2-cyanomethylimidazo[4,5-b]pyridine. Tuberculostatic investigations of obtained compounds
AUTHOR(S): Bukowski, Ludwik
CORPORATE SOURCE: Inst. Technol. Drug Anal., Med. Acad., Gdansk, 80-416, Pol.
SOURCE: Polish Journal of Pharmacology and Pharmacy (1986), 38(1), 91-8
CODEN: PJPPAA; ISSN: 0301-0244
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



AB 2-Cyanomethylimidazo[4,5-b]pyridine (I) was obtained by condensation of 2,3-diaminopyridine with NCCH₂CO₂Et. Hydrolysis, esterification, or derivatization of I gave II (R = Me, CO₂Me, CONH₂, CSNH₂, etc.). Knoevenagel condensation of I with aromatic and heterocyclic aldehydes yielded III (R₁ = Ph, PhCH₂CH, 4-O₂NC₆H₄, 2-furyl, etc.). Treatment of III with H₂S gave IV (R₁ = Ph, 3,4-(MeO)₂C₆H₃, 3,4-MeO(HO)C₆H₃, 2-furyl, 2-pyridyl). Tuberculostatic activity was shown by III (R₁ = CONH₂, CONHCH₂Ph, CSNH₂, C(NOH)NH₂) and IV when tested against Mycobacterium tuberculosis strain standard

RX(25) OF 62 ...AH → AQ



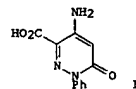
RX(25) RCT AH 107933-13-1

L11 ANSWER 31 OF 41 CASREACT COPYRIGHT 2005 ACS on STN (Continued)

RGT G 7783-06-4 H₂S
PRO AQ 107933-18-6
CAT 121-44-8 Et₃N

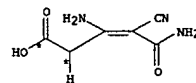
L11 ANSWER 32 OF 41 CASREACT COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 106:4964 CASREACT
TITLE: Activated nitriles in heterocyclic synthesis. A novel synthesis of pyridine and pyridazine derivatives
AUTHOR(S): Fahmy, Sherif Mahmoud; Mohareb, Rafat Hilal
CORPORATE SOURCE: Fac. Sci., Cairo Univ., Giza, Egypt
SOURCE: Synthesis (1985), (12), 1135-7
CODEN: SYNTBP; ISSN: 0039-7881
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

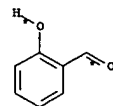


AB The dimerization of NCCH₂CONH₂ gave HO₂C(NH₂):C(CN)CONH₂ which cyclized with CH₂(COMe)PhCH:CR₂CN (R = cyano, CO₂Et), and EtOCH: C(CN)CO₂Et to give pyridine derivs. and with PhN₂+Cl⁻ to give the pyridazine I.

RX(7) OF 22 ...B + T → U



B



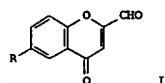
T



U

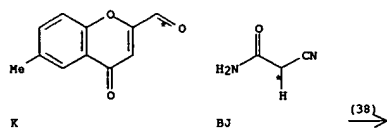
RX(7) RCT B 105626-24-2, T 90-02-8
PRO U 105626-30-0
CAT 110-89-4 Piperidine
SOL 68-12-2 DMF

L11 ANSWER 33 OF 41 CASREACT COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 106:4813 CASREACT
 TITLE: Synthesis and reactions of some 4-oxo-4H-1-benzopyran-2-carboxaldehydes
 AUTHOR(S): Sami, S. M.; Ibrahim, S. S.; Abdel-Halim, A. M.; Aly, Y. L.
 CORPORATE SOURCE: Fac. Educ., Ain Shams Univ., Cairo, Egypt
 SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1986), 25B(4), 384-9
 CODEN: IJSBDB; ISSN: 0376-4699
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI

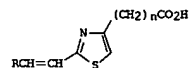


AB Some new 4-oxo-4H-1-benzopyran-2-carboxaldehydes were prepared; the conversion of the 2-carboxaldehyde group into 2-carbonitrile and 2-carboxylic acid groups was discussed. Unlike the general behavior of the 4-oxo-4H-1-benzopyrans towards some nucleophiles, where the reaction takes place with opening of the pyrone ring, I (R = Me, Cl) react with different nucleophiles, such as hydroxylamine hydrochloride, hydrazine, phenylhydrazine, and primary aromatic amines, to give the corresponding condensation products without the opening of pyrone ring. The only exception to this observation is the reaction of I (R = Me, Cl) with ethylenediamine where the opening of pyrone ring does not take place to give the expected 5,6-dihydropyrazine deriva. The reactions of I (R = Me, Cl) with active methylene compds., malonic acid, malonodinitrile, cyanoacetic acid, Et cyanoacetate, cyanoacetamide, and hippuric acid were also discussed.

RX(38) OF 98 ...K + BJ ==> BK

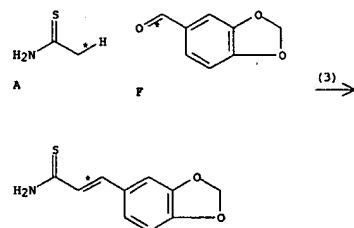


L11 ANSWER 34 OF 41 CASREACT COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 104:28388 CASREACT
 TITLE: Synthesis and pharmacological activities of 2-arylethylthiazole-4-acetic and 4-carboxylic acids
 AUTHOR(S): Bonina, F.; Guerrero, F.; Pappalardo, F.; Siracusa, M. A.; Catuso, A.; Trombadore, S.; Amico-Roxas, M.
 CORPORATE SOURCE: Ist. Chim. Tossicol., Univ. Catania, Catania, Italy
 SOURCE: Farmaco, Edizione Scientifica (1985), 40(11), 875-84
 CODEN: FRPSAX; ISSN: 0430-0920
 DOCUMENT TYPE: Journal
 LANGUAGE: Italian
 GI



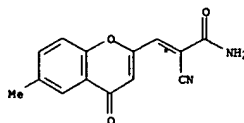
AB Eighteen title compds. (I; R = alkoxy-substituted aryl; n = 0 or 1) were prepared by condensation (in EtOH) of the corresponding 3-arylprop-2-ene thioamides, RCH=CHC(=S)NH2, with Et α-bromoacetoacetate [13176-46-0] (for I; n = 1) or Et bromopyruvate [70-23-5] (for I; n = 0), followed by alkaline hydrolysis. Pharmacol. testing in mice and rats showed 7 I to have moderate analgesic, antiinflammatory, and antipyretic activities; the most active compound was I (R = 3,4-methylenedioxypheyl; n = 0) [99661-55-9], whose activity was comparable to, or less than, that of the reference compds. Compared with previous results with halogen-substituted aryl compds. of the I type, the presence of the alkoxy groups decreased the toxicity, but also the analgesic, antiinflammatory, and antipyretic activities. The activities of I with n = 0 were comparable to those of I with n = 1, showing the lack of a specific requirement for the acetic acid side chain. The oral and i.p. LD50 values of I in mice were >800 and >500 mg/kg, resp.

RX(3) OF 9 A + F ==> G



G
 YIELD 76%

L11 ANSWER 33 OF 41 CASREACT COPYRIGHT 2005 ACS on STN (Continued)

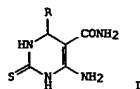


RX(38) ACT K 99851-63-5, BJ 107-91-5
 PRO BK 105391-83-1

L11 ANSWER 34 OF 41 CASREACT COPYRIGHT 2005 ACS on STN (Continued)

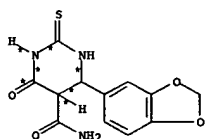
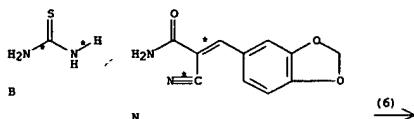
RX(3) ACT A 62-55-5, F 120-57-0
 PRO G 99661-62-8

L11 ANSWER 35 OF 41 CASREACT COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 103:104910 CASREACT
 TITLE: A simple synthesis of 4-amino-6-aryl-2-thioxotetra- and -hexahydropyrimidines
 AUTHOR(S): Lorente, Antonio; Garcia Navio, Jose L.; Lopez Perez, Jose C.; Soto, Jose L.
 CORPORATE SOURCE: Dep. Quim. Org., Univ. Alcalá de Henares, Madrid, Spain
 SOURCE: Synthesis (1985), (1), 89-92
 CODEN: SYNTBF; ISSN: 0039-7881
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



AB Cyclization of thiourea with (E)-RCH=C(CN)CONH₂ (R = Ph, p-tolyl, p-anisyl, p-ClC₆H₄, 2,4-Me₂CGH₃) gave 22-50% pyrimidinethiones I.

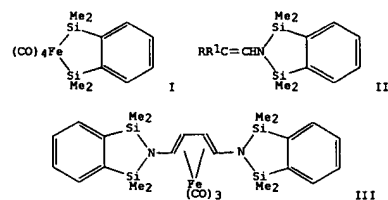
RX(6) OF 18 B + N ==> O



O

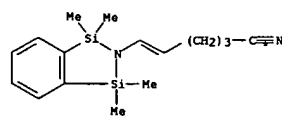
RX(6) RCT B 62-56-6, N 98011-39-3

L11 ANSWER 36 OF 41 CASREACT COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 102:149346 CASREACT
 TITLE: Silyliron carbonyl complexes in organic synthesis: selective conversion of nitriles into N,N-bis(silyl) enamines
 AUTHOR(S): Corriu, Robert J. P.; Moreau, Joel J. E.; Pataud-Sat, Magali
 CORPORATE SOURCE: Lab. Organometall., Univ. Sci. Tech. Languedoc, Montpellier, F-34060, Fr.
 SOURCE: Organometallics (1985), 4(4), 623-9
 CODEN: ORGN7; ISSN: 0276-7333
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



AB Treating o-(Me₂SiH)₂CGH₄ with Fe(CO)₅ gave 50-70% of the chelated ferradisila complex I. I reacted photochem. with nitriles RR'CHCN (R = R' = H, Me, Ph; R' = Me, Ph, CH₂Ph, SiMe₃, cyano, cyanoalkyl, o-NCCGH₄, Cl, MeO, EtO₂C, etc.) to give 30-95% silyl enamines E- and Z-II. Acidic hydrolysis of II (R = R' = H, Me, Ph; R' = Me, Ph, NC(CH₂)₃, EtO₂C) gave the aldehydes RR'CHCHO. II are stable in the presence of electrophiles and nucleophiles and can be used as protected aldehydes. I reacted with II (R = H, R' = CH₂CN) or NCCH₂CH₂CN to give the iron diaminodiene complex III in 70 or 50% yield, resp.

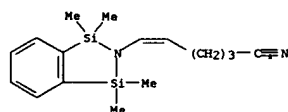
RX(28) OF 163 ...AF + AG ==> BB + BO



AF

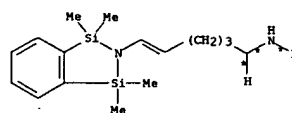
L11 ANSWER 35 OF 41 CASREACT COPYRIGHT 2005 ACS on STN (Continued)
 RGT P 7440-23-5 Na
 PRO O 98011-33-7
 SOL 67-63-0 Me₂CHOH

L11 ANSWER 36 OF 41 CASREACT COPYRIGHT 2005 ACS on STN (Continued)

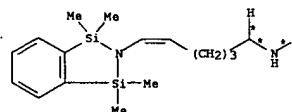


AG

(28)



BN



BO

RX(28) RCT AF 78108-79-9, AG 78108-80-2

STAGE(1)
 RGT BP 16853-85-3 LiAlH₄
 SOL 60-29-7 Et₂O

STAGE(2)
 RGT BQ 15490-42-3 Butanedioic acid, 2,3-dihydroxy- (2R,3R)-, potassium sodium salt
 SOL 7732-18-5 Water
 PRO BN 95192-90-8, BO 95192-91-9

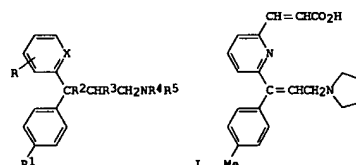
L11 ANSWER 37 OF 41 CASREACT COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 100:6345 CASREACT
 TITLE: Aromatic compounds
 INVENTOR(S): Coker, Geoffrey George; Findlay, John William Addison
 PATENT ASSIGNEE(S): Wellcome Foundation Ltd., UK
 SOURCE: Eur. Pat. Appl., 66 pp.
 CODEN: EPXOXW
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 2
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 85959	A2	19830817	EP 1983-101036	19830203
EP 85959	A3	19840718		
EP 85959	B1	19850419		
R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE				
US 4501893	A	19850226	US 1983-462872	19830201
US 4562258	A	19851231	US 1983-462874	19830201
DK 8300436	A	19830805	DK 1983-436	19830203
DK 164662	B	19920727		
DK 164662	C	19921214		
FI 8300380	A	19830805	FI 1983-380	19830203
FI 82450	B	19901130		
FI 82450	C	19910311		
NO 8300368	A	19830805	NO 1983-368	19830203
NO 162556	B	19891009		
NO 162556	C	19900117		
AU 8310982	A1	19830811	AU 1983-10982	19830203
AU 555083	B2	19860911		
GB 2114565	A1	19830824	GB 1983-2971	19830203
GB 2114565	B2	19850626		
JP 58164557	A2	19830929	JP 1983-16847	19830203
JP 01053671	B4	19891115		
HU 27600	O	19831028	HU 1983-377	19830203
HU 189223	B	19860630		
ES 519491	A1	19840401	ES 1983-519491	19830203
ZA 8300737	A	19840926	ZA 1983-737	19830203
CS 235306	B2	19850515	CS 1983-754	19830203
PL 140708	B1	19870530	PL 1983-240412	19830203
PL 140809	B1	19870530	PL 1983-245841	19830203
PL 140810	B1	19870530	PL 1983-245842	19830203
PL 140811	B1	19870530	PL 1983-245843	19830203
PL 140812	B1	19870530	PL 1983-245844	19830203
PL 141639	B1	19870831	PL 1983-245845	19830203
EP 249950	A1	19871223	EP 1987-108671	19830203
EP 249950	B1	19910619		
R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE				
IL 67829	A1	19880630	IL 1983-67829	19830203
SU 1436871	A3	19881107	SU 1983-355527	19830203
IL 78419	A1	19890131	IL 1983-78419	19830203
AT 42282	E	19890515	AT 1983-101036	19830203
AT 64596	E	19910715	AT 1987-108671	19830203
DD 209446	A5	19840509	DD 1983-247730	19830204
CA 1249830	A1	19890207	CA 1983-420912	19830204
ES 523414	A1	19841001	ES 1983-523414	19830620

L11	ANSWER 37 OF 41	CASREACT	COPYRIGHT	2005 ACS	ON STN	(Continued)
ES 523415	A1	19841001	ES	1983-523415	19830620	
ES 523416	A1	19841001	ES	1983-523416	19830620	
ES 523417	A1	19841001	ES	1983-523417	19830620	
ES 523418	A1	19841001	ES	1983-523418	19830620	
SU 1301312	A3	19870330	SU	1983-3652410	19831017	
SU 1416057	A3	19880807	SU	1983-3652703	19831017	
SU 1447280	A3	19881223	SU	1983-3652921	19831017	
SU 1516009	A3	19891015	SU	1983-3654489	19831017	
CS 235347	B2	19850515	CS	1984-2018	19840321	
CS 235348	B2	19850515	CS	1984-2019	19840321	
CS 235349	B2	19850515	CS	1984-2020	19840321	
CS 235350	B2	19850515	CS	1984-2021	19840321	
US 4650807	A	19870317	US	1985-753791	19850708	
US 4657918	A	19870414	US	1985-779877	19850925	
JP 63033343	A2	19880213	JP	1987-106133	19870428	
JP 03048181	B4	19910723				
NO 8704330	A	19830805	NO	1987-4330	19871016	
NO 172341	B	19930329				
NO 172341	C	19930707				
JP 01079153	A2	19890324	JP	1988-135352	19880601	
JP 02051897	B4	19901108				
CA 1275102	A2	19901009	CA	1988-575487	19880823	
JP 01301661	A2	19891205	JP	1989-98616	19890418	
JP 04000068	B4	19920106				

PRIORITY APPLN. INFO.:

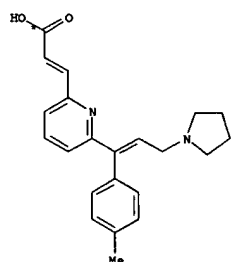
GI



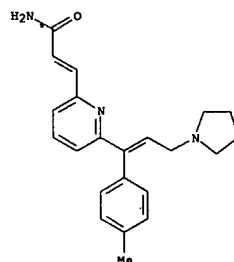
AB Amines I (X = N, CH; R = CO2H, carboxyalkyl, carboxyalkenyl; R1 = H, halogen, OH, cyano, acyloxy, alkoxy, alkyl, haloalkyl; R2, R3 = H; R2R3 = bond; NR4R5 = amino) were prepared (E,E)-II was prepared from

L11 ANSWER 37 OF 41 CASREACT COPYRIGHT 2005 ACS on STN (Continued)
 2,6-dibromopyridine, 4-MeC6H4CN, EtO2CH2P(O)(OEt)2, and (2-pyrrolidinoethyl)triphenylphosphonium bromide in 5 steps. II has an antihistaminic pKa of 8.6.

RX(6) OF 43 ...K ==> L



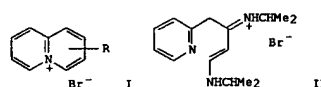
(6) →



L

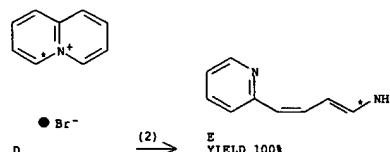
RX(6) RCT K 87848-99-5
 PRO L 87849-16-9

L11 ANSWER 38 OF 41 CASREACT COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 99:88022 CASREACT
 TITLE: Reactions of halogenoquinolinium bromides with aniline, isopropylamine and liquid ammonia
 AUTHOR(S): Sanders, G. M.; Van Dijk, M.; Van der Plas, H. C.; Konijn, M.; Stam, C. H.
 CORPORATE SOURCE: Lab. Org. Chem., Agric. Univ., Wageningen, Neth.
 SOURCE: Journal of Heterocyclic Chemistry (1983), 20(2), 407-14
 CODEN: JHCTAC; ISSN: 0022-152X
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



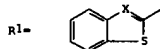
AB The reactions of quinolinium bromides (I, R = H, Br) with PhNH2, Me2CHNH2 and NH2(1) were investigated. With PhNH2, I (R = 2-Br, 4-Br) undergoes substitution, whereas I (R = 1-Br, 3-Br) do not react at all. With NH3 all bromo derivs. and the parent compound react with ring opening. This diversity in the reaction course is explained in terms of the hard-soft acid-base principle. I (R = 2-Br) reacts with Me2CHNH2 to give I (R = 2-Me2CHNH). Two mols. of Me2CHNH2 are involved in this substitution, as intermediate imine II was isolated. The structure of II was confirmed by x-ray crystal structure anal.

RX(2) OF 12 D ==> E...



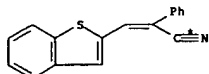
RX(2) RCT D 1004-95-1
 RGT F 7664-41-7 NH3
 PRO E 06018-42-0

L11 ANSWER 39 OF 41 CASREACT COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 99:22366 CASREACT
 TITLE: Investigation on some (E)- and (Z)-3-heterocyclic-substituted-2-phenylacrylic acids
 AUTHOR(S): Belgodere, Elena; Bossio, Ricardo; Cencioni, Roberto; Pepino, Roberto
 CORPORATE SOURCE: Cent. Stud. Chim. Strutt. Composti Eterociclici Loro Appl., CNR, Florence, 50121, Italy
 SOURCE: Journal of Heterocyclic Chemistry (1983), 20(1), 5-7
 CODEN: JHCTAD; ISSN: 0022-152X
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI

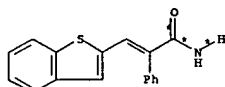


AB (E)- And (Z)-RCH:CPHCO₂H (R = 2-thiazolyl) and (E)-RCH:CPHCO₂H (I; R = R1, X = N,CH) were prepared by condensation of RH with PhCH₂CO₂H. (Z)-I (R = R1, X = N) was prepared by hydrolysis of (Z)-RICH:CPH₂CN but careful hydrolysis of (Z)-RICH:CPH₂CN (X = CH) gave only (E)- and (Z)-RICH:CPHCONH₂. S And Z configurations were distinguished by their spectra.

RX(1) OF 2 A ==> B



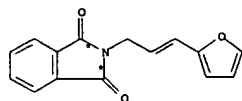
(1) →



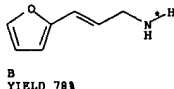
RX(1) RCT A 86213-36-7
 RGT C 7647-01-0 HC1
 PRO B 86213-37-8

L11 ANSWER 40 OF 41 CASREACT COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 95:42789 CASREACT
 TITLE: Highly stereoselective route to (E)-allyl amines via vinyltri-n-butylphosphonium salts (Schweizer reaction)
 AUTHOR(S): Meyers, A. I.; Lawson, Jon P.; Carver, David R.
 CORPORATE SOURCE: Dep. Chem., Colorado State Univ., Fort Collins, CO, 80523, USA
 SOURCE: Journal of Organic Chemistry (1981), 46(15), 3119-23
 CODEN: JOCEAH; ISSN: 0022-3263
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB The reaction of vinyltri-n-butylphosphonium salts, aldehydes, and sodiophthalimide in THF gave good yields of the allylic phthalimides with high E-stereoselectivity (75-100%). The use of the vinyltriphenylphosphonium salts (Schweizer reaction) gave the allyl phthalimide with the Z isomer predominating. A study of the phthalimide cation and the effect of added Li salt showed some reversal in the olefin geometry but in general the selectivity was only 3:1.

RX(1) OF 4 A ==> B



(1) →

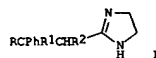


YIELD 78%

RX(1) RCT A 77629-11-9
 RGT C 302-01-2 N2H4
 PRO B 300687-38-1

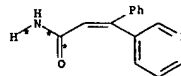
L11 ANSWER 39 OF 41 CASREACT COPYRIGHT 2005 ACS on STN (Continued)

L11 ANSWER 41 OF 41 CASREACT COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 94:30641 CASREACT
 TITLE: Cyclic guanidines. X. Synthesis of 2-(2,2-disubstituted ethenyl- and ethyl)-2-imidazolines as potent hypoglycemics
 AUTHOR(S): Ishikawa, Fumiyoshi
 CORPORATE SOURCE: Res. Inst., Daiichi Seiyaku Co., Ltd., Tokyo, 132, Japan
 SOURCE: Chemical & Pharmaceutical Bulletin (1980), 28(5), 1394-402
 CODEN: CPBTAL; ISSN: 0009-2363
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI

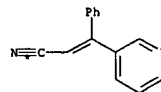


AB 2-(2,2-Disubstituted ethenyl- and ethyl)-2-imidazoline derivs. I (R = Me, Ph, pyridyl; R1-R2 = H; R1R2 = bond) were prepared by direct cyclization of RCPH:CHC(:NR3)OEt (R3 = H, CHMe2) with ethylenediamine. The stereoisomers, (Z)- and (E)-RCPH:CHC(:NR3)OEt, RCPH:CHCN RCPH:CHCONH₂, RCPH:CHC(:NH)OEt, and I (R = pyridyl, R1R2 = bond) were isolated. Their structures are discussed. I showed potent hypoglycemic activity.

RX(20) OF 223 ...AB ==> AA...



(20) →



AA
 YIELD 69%

RX(20) RCT AB 344422-02-2
 PRO AA 184419-56-5

10/ 821,906

=> d his

(FILE 'HOME' ENTERED AT 11:47:31 ON 03 AUG 2005)

FILE 'REGISTRY' ENTERED AT 11:47:36 ON 03 AUG 2005

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L2 STRUCTURE UPLOADED
L3 STRUCTURE UPLOADED
L4 STRUCTURE UPLOADED
L5 50 S L1 SAMPLE
L6 41960 S L1 FULL
L7 10 S L2 FUL SUB=L6
L8 2481 S L3 FUL SUB=L6
L9 0 S L4 FUL SUB=L6

FILE 'CASREACT' ENTERED AT 11:52:42 ON 03 AUG 2005

L10 205 S L7 OR L8
L11 41 S L10 AND (DEPROTECT? OR HYDROLY? OR CLEAV?)
L12 3 S L10 AND ((ACID CHLORIDE) OR (ACID IMIDAZOL?))

=> s l12 not l11

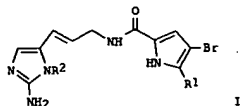
L13 3 L12 NOT L11

=> d l13 1- ibib abs fhit

YOU HAVE REQUESTED DATA FROM 3 ANSWERS - CONTINUE? Y/(N):y

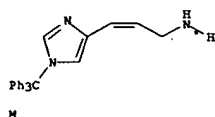
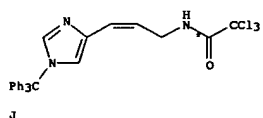
L13 ANSWER 1 OF 3 CASREACT COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 127:95441 CASREACT
 TITLE: Synthesis of marine 2-aminoimidazole metabolites:
 hymenidin, oroidin, and keramidine
 AUTHOR(S): Daninos-Zeghal, Sophie; Al Mourabit, Ali; Ahond,
 Alain; Poupat, Christiane; Potier, Pierre
 CORPORATE SOURCE: Inst. Chimie des Substances Naturelles CNRS,
 Gif-sur-Yvette, 91198, Fr.
 SOURCE: Tetrahedron (1997), 53(22), 7605-7614
 PUBLISHER: Elsevier
 DOCUMENT TYPE: Journal
 LANGUAGE: French
 GI



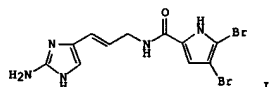
AB Through a general synthetic scheme, hymenidin [I; R1 = R2 = H (II)], oroidin [I; R1 = Br, R2 = H (III)] and keramidine [I; R1 = H, R2 = Me (IV)], all marine 2-aminoimidazole metabolites, were prepared. An improved synthesis of III and the first syntheses of II and IV were obtained over seven steps from 1H-imidazole-4-methanol.

RX(3) OF 39 ...J ==> M...



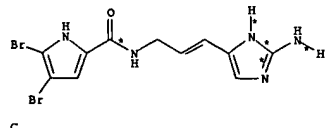
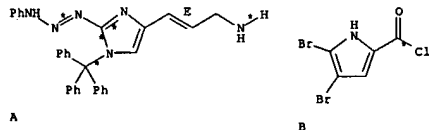
L13 ANSWER 2 OF 3 CASREACT COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 108:56424 CASREACT
 TITLE: Synthesis of oroidine
 AUTHOR(S): De Wanteuil, Guillaume; Ahond, Alain; Poupat,
 Christiane; Thoison, Odile; Potier, Pierre
 CORPORATE SOURCE: Inst. Chim. Subst. Nat., CNRS, Gif-sur-Yvette, 91190,
 Fr.
 SOURCE: Bulletin de la Societe Chimique de France (1986), (5),
 813-16
 CODEN: BSCFAS; ISSN: 0037-8968
 DOCUMENT TYPE: Journal
 LANGUAGE: French
 GI



AB Oroidine (I), a product isolated from several sponges, has been synthesized following two different routes using the same starting material: 4(5)-(hydroxymethyl)imidazole.

RX(1) OF 31 ...A + B ==> C



RX(1) RCT A 112547-06-5, B 40160-15-4
 RGT D 7647-01-0 HCl
 PRO C 34649-22-4
 SOL 75-09-2 CH2Cl2, 7732-18-5 Water

L13 ANSWER 1 OF 3 CASREACT COPYRIGHT 2005 ACS on STN (Continued)

RX(3) RCT J 132553-81-2
 RGT N 1310-73-2 NaOH
 PRO M 138408-51-2
 SOL 7732-18-5 Water, 123-91-1 Dioxane
 REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 2 OF 3 CASREACT COPYRIGHT 2005 ACS on STN (Continued)

L13 ANSWER 3 OF 3 CASREACT COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

TITLE:

INVENTOR(S):

PATENT ASSIGNER(S):

SOURCE:

DOCUMENT TYPE:

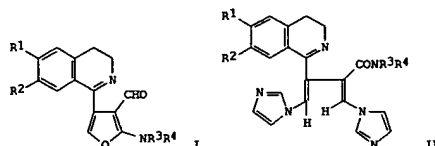
LANGUAGE:

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3603194	A1	19870806	DE 1986-3603194	19860203
EP 234329	A1	19870902	EP 1987-101292	19870130
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
DK 8700526	A	19870804	DK 1987-526	19870202
FI 8700435	A	19870804	FI 1987-435	19870202
NO 8700408	A	19870804	NO 1987-408	19870202
JP 62185086	A2	19870813	JP 1987-22278	19870202
DD 260067	A5	19880914	DD 1987-299666	19870202
ZA 8700730	A	19881026	ZA 1987-730	19870202
HU 47100	A2	19890130	HU 1987-351	19870202
AU 8768235	A1	19870806	AU 1987-68235	19870203
PRIORITY APPLN. INFO.:			DE 1986-3603194	19860203

GI



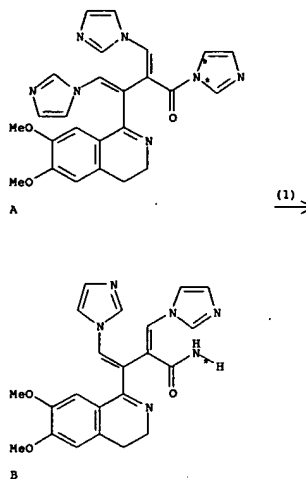
AB Formylfurans I [R1, R2 = H, MeO, SH, NH2; R3, R4 = H or (un)substituted C1-12 aliphatic; R3R4N = heterocyclyl optionally with further N, O, or S hetero atoms] and their salts, useful in treating coronary heart disease or cerebral metabolic disturbances and thus useful as Ca antagonists and antiarrhythmics and in treating angina pectoris, heart infarction, cerebral insufficiency, hypoxia and improving circulation (no data), were prepared by cyclizing amides II in the presence of H2O and proton acids and optional conversion into salts or interconversion of salts.
4-(3,4-Dihydro-6,7-dimethoxy-1-isoquinolinyl)-3-furancarboxylic acid-HCl reacted with N,N'-dicarbonyldiimidazole to give 83% 1,4-di(1-imidazolyl)-3-[(3,4-dihydro-6,7-dimethoxy)-1-isoquinolinyl]butadiene-2-carboxylic

L13 ANSWER 3 OF 3 CASREACT COPYRIGHT 2005 ACS on STN (Continued)

acid imidazolide, amidation of which with NH3-satd.

CH2Cl2 gave 93% the corresponding 2-carboxamide. Cyclization of this with 2N HCl in EtOH gave 82% 2-(2-furanylmethylamino)-4-[(3,4-dihydro-6,7-dimethoxy)-1-isoquinolinyl]-3-furancarboxaldehyde.

RX(1) OF 2 A → B



RX(1) RCT A 110857-59-5
PRO B 110857-60-8
CAT 7664-41-7 NH3, 37555-63-8 Lithium, (dibromomethyl)-